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*Published in:*  
Journal of functional analysis

*DOI:*  
[10.1016/j.jfa.2003.06.005](https://doi.org/10.1016/j.jfa.2003.06.005)

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*Document Version*  
Publisher's PDF, also known as Version of record

*Publication date:*  
2004

[Link to publication in University of Groningen/UMCG research database](#)

*Citation for published version (APA):*

Dijksma, A., Langer, H., & Shondin, Y. (2004). Rank one perturbations at infinite coupling in Pontryagin spaces. *Journal of functional analysis*, 209(1), 206-246. <https://doi.org/10.1016/j.jfa.2003.06.005>

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# Rank one perturbations at infinite coupling in Pontryagin spaces<sup>☆</sup>

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Received 9 January 2003; accepted 12 June 2003

Communicated by D. Sarason

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## Abstract

In this paper we relate the operators in the operator representations of a generalized Nevanlinna function  $N(z)$  and of the function  $-N(z)^{-1}$  under the assumption that  $z = \infty$  is the only (generalized) pole of nonpositive type. The results are applied to the  $Q$ -function for  $S$  and  $H$  and the  $Q$ -function for  $S$  and  $H^\infty$ , where  $H$  is a self-adjoint operator in a Pontryagin space with a cyclic element  $w$ ,  $H^\infty$  is the self-adjoint relation obtained from  $H$  and  $w$  via a rank one perturbation at infinite coupling, and  $S$  is the symmetric operator given by  $S = H \cap H^\infty$ .

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MSC: 47B50; 47B25; 47A06; 34L99; 33C10

**Keywords:** Pontryagin space; Hilbert space; Defect function;  $Q$ -function; Generalized Nevanlinna function; Infinite coupling; Rank one perturbation; Symmetric operator; Self-adjoint linear relation; Extension theory

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<sup>☆</sup> The research for this paper was supported by the Netherlands Organization for Scientific Research NWO (grant 047-008-008), the Russian Foundation for Basic Research RFBR (grant N 0001-00544), and the Research Training Network HPRN-CT-2000-00116 of the European Union.

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## 1. Introduction

**1.1.** First we recall some notions and facts from the extension theory of symmetric operators in Pontryagin spaces; for the proofs we refer to [9,18,19]. Let  $S$  be a symmetric (not necessarily densely defined) operator in a Pontryagin space  $(\Pi_\kappa, \langle \cdot, \cdot \rangle)$ ,  $\kappa \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$ , with defect index  $(1, 1)$  and let  $A$  be a self-adjoint extension of  $S$  in  $\Pi_\kappa$ ;  $A$  can be an operator or a linear relation with nonempty resolvent set  $\rho(A)$ . A *defect function*  $\varphi(z)$  associated with  $S$  and  $A$  is a holomorphic function on  $\rho(A)$  with values in  $\Pi_\kappa$  and the properties  $\varphi(z) \in \ker(S^* - z)$  and

$$\varphi(z) - \varphi(\zeta) = (z - \zeta)(A - z)^{-1}\varphi(\zeta), \quad z, \zeta \in \rho(A). \quad (1.1)$$

Then the *Q-function* associated with  $S$  and  $A$  is a holomorphic function  $N(z)$  on  $\rho(A)$  which satisfies the relation

$$\frac{N(z) - N(\zeta)^*}{z - \zeta^*} = \langle \varphi(z), \varphi(\zeta) \rangle, \quad z, \zeta \in \rho(A); \quad (1.2)$$

in particular,  $N(z)^* = N(z^*)$ ,  $z \in \rho(A)$ . This function is uniquely defined up to a real constant. If  $z_0 \in \rho(A)$  is fixed, it is given by

$$N(z) = N(z_0^*) + (z - z_0) \langle \varphi(z), \varphi(z_0) \rangle,$$

that is, with  $u = \varphi(z_0)$

$$N(z) = N(z_0^*) + (z - z_0^*) \langle (I + (z - z_0)(A - z)^{-1})u, u \rangle, \quad z \in \rho(A). \quad (1.3)$$

If the *minimality condition*

$$\Pi_\kappa = \overline{\text{span}}\{\varphi(z) \mid z \in \rho(A)\} \quad (1.4)$$

is satisfied, it belongs to the class  $\mathcal{N}_\kappa$  of *generalized Nevanlinna functions with  $\kappa$  negative squares*. Recall that  $\mathcal{N}_\kappa$  is the set of all functions  $N(z)$  which are defined and meromorphic in  $\mathbb{C}^+ \cup \mathbb{C}^-$ , such that  $N(z)^* = N(z^*)$  and that the kernel

$$\mathbf{N}_N(z, \zeta) = \frac{N(z) - N(\zeta)^*}{z - \zeta^*}, \quad z, \zeta \in \rho(N),$$

has  $\kappa$  negative squares; here  $\rho(N)$  denotes the *domain of holomorphy* of  $N(z)$ . If  $\kappa = 0$ , the class  $\mathcal{N}_0$  consists of all *Nevanlinna functions*, these are the functions  $N(z)$  which are holomorphic in  $\mathbb{C}^+ \cup \mathbb{C}^-$  and such that  $N(z)^* = N(z^*)$  and

$$\frac{\text{Im } N(z)}{\text{Im } z} \geq 0, \quad z \in \mathbb{C}^+ \cup \mathbb{C}^-.$$

Also, conversely, each function  $N(z) \in \mathcal{N}_\kappa$  is a *Q-function* associated as above with a symmetric operator  $S$  in some Pontryagin space  $\Pi_\kappa$  and a self-adjoint extension  $A$  of  $S$  in  $\Pi_\kappa$ , which are uniquely determined up to unitary equivalence if the minimality

condition (1.4) is satisfied. This condition also implies that  $\rho(A) = \rho(N)$ . In this situation we write for short

$$N(z) \sim S, A \text{ in } \Pi_\kappa,$$

always assuming that (1.4) holds. If  $N(z) \sim S, A$  in  $\Pi_\kappa$  then  $S$  is a densely defined symmetric operator if and only if the function  $N(z) \in \mathcal{N}_\kappa$  has the properties

$$(a) \lim_{y \rightarrow +\infty} y \operatorname{Im} N(iy) = +\infty, \quad (b) \lim_{y \rightarrow \infty} y^{-1} N(iy) = 0. \quad (1.5)$$

In fact, (a)  $\Leftrightarrow \overline{\operatorname{dom}} S = \overline{\operatorname{dom}} A$ , and (b)  $\Leftrightarrow \overline{\operatorname{dom}} A = \Pi_\kappa$ . This holds, in particular, also for  $\kappa = 0$  in which case  $\Pi_0$  is a Hilbert space.

A function  $N(z) \in \mathcal{N}_\kappa$  has  $\kappa$  poles or generalized poles of nonpositive type, counted according to their multiplicities, in the closed upper half-plane, see [20,22]. If  $z = \infty$  is the only pole of nonpositive type or generalized pole of nonpositive type of the generalized Nevanlinna function  $N(z)$  (or, equivalently (see [21]), the spectrum of  $A$  in the operator representation of  $N(z)$  is real and all the spectral points of  $A$  in  $\mathbb{R}$  are of positive type), then, according to [2,19],  $N(z)$  is characterized by a representation

$$N(z) = c(z)^m N_0(z) + p(z), \quad c(z) := (z - z_0)(z - z_0^*), \quad (1.6)$$

where  $z_0 \in \mathbb{C} \setminus \mathbb{R}$ ,  $m \in \mathbb{N}_0$ ,  $N_0(z) \in \mathcal{N}_0$ , and  $p(z)$  is a real polynomial. Representation (1.6) can always be chosen such that it is *irreducible*, that is, has the properties

$$m \text{ is minimal, } \lim_{y \rightarrow \infty} y^{-1} N_0(iy) = 0, \quad \operatorname{Re} N_0(i) = 0,$$

and then this representation is unique. Here the last equality is a normalization condition on  $N_0(z)$ . If  $m > 0$ , then the minimality of  $m$  is equivalent to (1.5)(a) with  $N_0(z)$  instead of  $N(z)$ .

In this paper we study functions from the slightly smaller class  $\mathcal{N}_\kappa^\infty$ . By definition this is the class of functions  $N(z) \in \mathcal{N}_\kappa$  with irreducible Representation (1.6) in which, also when  $m = 0$ , (1.5) holds for  $N_0(z)$  instead of  $N(z)$ . Thus,  $N(z) \in \mathcal{N}_\kappa^\infty$  if and only if  $N(z) \in \mathcal{N}_\kappa$  has a representation of form (1.6), where the Nevanlinna function  $N_0(z)$  has the properties

$$\lim_{y \rightarrow +\infty} y \operatorname{Im} N_0(iy) = +\infty, \quad \lim_{y \rightarrow \infty} y^{-1} N_0(iy) = 0, \quad \operatorname{Re} N_0(i) = 0. \quad (1.7)$$

Functions of form (1.6) with  $m = 0$  and

$$\lim_{y \rightarrow +\infty} y \operatorname{Im} N_0(iy) < +\infty, \quad \lim_{y \rightarrow \infty} y^{-1} N_0(iy) = 0$$

are studied in [4].

**1.2.** We outline the contents of the paper. In Section 2 we consider a self-adjoint operator  $H$  in a Pontryagin space  $\Pi_\kappa$  with cyclic element  $w$  and form the rank one

perturbation  $H + \alpha \langle \cdot, w \rangle w$ ,  $\alpha \in \mathbb{R}$ . Infinite coupling by letting  $\alpha \rightarrow \infty$  yields a self-adjoint relation  $H^\infty$ . If  $S$  is the symmetric operator  $S := H \cap H^\infty$ , then the  $Q$ -functions  $Q(z) \sim S, H$  and  $Q^\infty(z) \sim S, H^\infty$  in  $\Pi_\kappa$  satisfy the relation  $Q^\infty(z) = -Q(z)^{-1}$ , see Theorem 2.1. Recall that if  $N(z) \in \mathcal{N}_\kappa$  then also the function<sup>1</sup>  $\hat{N}(z) := -N(z)^{-1}$  belongs to the same class  $\mathcal{N}_\kappa$  and the resolvents of the operators appearing in the representations are one-dimensional perturbations of each other, see for example [23].

In Section 3 we show that in representation (1.3) of a function  $\hat{N}(z) \in \mathcal{N}_\kappa$ :

$$\hat{N}(z) = \hat{N}(z_0^*) + (z - z_0^*) \langle (I + (z - z_0)(\hat{A} - z)^{-1})u, u \rangle, \quad z \in \rho(\hat{A}),$$

$\hat{A}$  is not an operator but a linear relation if and only if for the inverse function  $N(z) = -\hat{N}(z)^{-1}$  the representation corresponding to (1.3) simplifies to

$$N(z) = \langle (A - z)^{-1}w, w \rangle \quad (1.8)$$

with some element  $w \in \Pi_\kappa$ .

The main results of this paper, Theorems 4.2 and 5.1, concern the following question: Given a function  $N(z) \in \mathcal{N}_\kappa$  such that  $\hat{N}(z)$  belongs to  $\mathcal{N}_\kappa^\infty$  and has the irreducible representation (1.6):

$$\hat{N}(z) = c(z)^m \hat{N}_0(z) + p(z).$$

Then, according to what was said above, there exist a symmetric operator  $S$  and a self-adjoint extension  $A$  in a Pontryagin space  $\Pi_\kappa$ , a symmetric operator  $\hat{S}$ , a self-adjoint extension  $\hat{A}$  in a Pontryagin space  $\hat{\Pi}_\kappa$ , and a symmetric operator  $S_0$  and a self-adjoint extension  $A_0$  in a Hilbert space  $\mathcal{H}_0$  such that

$$N(z) \sim S, A \text{ in } \Pi_\kappa, \quad \hat{N}(z) \sim \hat{S}, \hat{A} \text{ in } \hat{\Pi}_\kappa, \quad \hat{N}_0(z) \sim S_0, A_0 \text{ in } \mathcal{H}_0. \quad (1.9)$$

What are the connections between these operators or relations and between the spaces? We mention already here that the spaces  $\Pi_\kappa$  and  $\hat{\Pi}_\kappa$  and also  $S$  and  $\hat{S}$  can be chosen to coincide, which implies that  $A$  and  $\hat{A}$  are self-adjoint extensions of the same symmetric operator.

In Section 4, we specialize to functions  $N(z) \in \mathcal{N}_\kappa$  of form (1.8) for which the corresponding functions  $\hat{N}(z)$  belong to  $\mathcal{N}_\kappa^\infty$ . In Theorem 4.2, we give an analytic and an operator characterization of such functions  $N(z)$  and an operator characterization of  $\hat{N}(z)$ : The analytic description of  $N(z)$  concerns its asymptotic behavior at  $z = \infty$ ; the operator description of  $N(z)$  concerns the smoothness of the element  $w$ :  $w \in \text{dom } A^{m+q-1} \setminus \text{dom } A^{m+q}$  and the signature of the space  $\mathcal{L} = \text{span}\{w, Aw, \dots, A^{m+q-1}w\}$  in the space  $\Pi_\kappa$  in terms of  $m, q \in \mathbb{N}_0$ ,  $m + q > 1$ . Finally,

<sup>1</sup> When dealing with the inverse of a function we tacitly assume that the function is not identically zero.

this subspace  $\mathcal{L}$  is the root space at  $z = \infty$  of the linear relation  $\widehat{A}$  appearing in the operator characterization of  $\widehat{N}(z)$ .

In Section 5, we apply these results to the self-adjoint operator  $H$  with cyclic element  $w$  and the self-adjoint relation  $H^\infty$  obtained by infinite coupling in Section 2. We mention that in the case  $\kappa = 1$  the signature of the root subspace of  $H^\infty$  at  $\infty$  was studied in [5].

As an example and motivation for this paper we consider in the next subsection of this introduction the Bessel operator. In the last subsection we give some definitions and basic facts which will be used in the sequel.

The singular perturbation studied in our earlier paper [10] led essentially to generalized Nevanlinna functions of class  $\mathcal{N}_\kappa^\infty$  with irreducible representation (1.6) in which  $m = \kappa$  and hence  $\deg p(z) \leq 2m$ . However, in [10] also a more explicit description of the underlying models and the free parameters was given. In another paper such models will also be considered for functions of  $\mathcal{N}_\kappa^\infty$  with  $m \neq \kappa$ .

**1.3.** As a motivation for these studies we consider the Bessel differential expression of order  $\nu \in \mathbb{R}$

$$l_\nu := -\frac{d^2}{dx^2} + \frac{\nu^2 - \frac{1}{4}}{x^2} \quad \text{on } (0, 1] \quad (1.10)$$

in the Hilbert space  $\mathcal{H}_0 = L^2(0, 1)$ ; for details see [7] and also [11], where the expression is considered on the interval  $(0, \infty)$ . At the regular endpoint 1 we fix the boundary condition  $y(1) = 0$ . At the singular endpoint 0 the expression is limit circle if  $|\nu| < 1$  and limit point if  $|\nu| \geq 1$ . Thus the minimal operator  $L_\nu$  associated with  $l_\nu$  in  $\mathcal{H}_0$  is symmetric and has defect index  $(1, 1)$  if  $|\nu| < 1$  and it is self-adjoint if  $|\nu| \geq 1$ . For the sake of simplicity we restrict  $\nu$  to  $\nu \in \Delta_0 := (0, 1)$  and  $\nu \in \Delta_1 := (1, \infty) \setminus \mathbb{N}$ .

If  $\nu \in \Delta_0$ , the function

$$\varphi_\nu^\infty(x, z) = \frac{\pi}{2 \sin \pi \nu} z^{\nu/2} x^{1/2} \left( \frac{J_{-\nu}(\sqrt{z})}{J_\nu(\sqrt{z})} J_\nu(x\sqrt{z}) - J_{-\nu}(x\sqrt{z}) \right)$$

belongs to  $L^2(0, 1)$  and satisfies the Bessel differential equation  $l_\nu y - zy = 0$ , hence

$$\varphi_\nu^\infty(\cdot, z) \in \ker(L_\nu^* - z). \quad (1.11)$$

It turns out to be a defect function with corresponding  $Q$ -function

$$Q_\nu^\infty(z) = Q_\nu^\infty(z_0^*) + (z - z_0^*) \langle \varphi_\nu^\infty(\cdot, z), \varphi_\nu^\infty(\cdot, \zeta) \rangle_{L^2(0,1)} = -\frac{\pi}{2 \sin \pi \nu} z^\nu \frac{J_{-\nu}(\sqrt{z})}{J_\nu(\sqrt{z})},$$

where  $z_0 \in \rho(Q_\nu^\infty)$ . The formula implies that

$$\rho(Q_\nu^\infty) = \mathbb{C} \setminus \{z \in \mathbb{C} \mid z^{-\nu/2} J_\nu(\sqrt{z}) = 0\}$$

and hence the choice  $z_0 = 0$  is admissible. It can also be shown that

$$\varphi_v(x, z) = \frac{\varphi_v^\infty(x, z)}{Q_v^\infty(z)} = z^{-v/2} x^{1/2} \left( \frac{J_v(\sqrt{z})}{J_{-v}(\sqrt{z})} J_{-v}(x\sqrt{z}) - J_v(x\sqrt{z}) \right) \quad (1.12)$$

is a defect function and that the corresponding  $Q$ -function is given by

$$Q_v(z) = -Q_v^\infty(z)^{-1} = -\frac{2 \sin \pi v}{\pi} z^{-v} \frac{J_v(\sqrt{z})}{J_{-v}(\sqrt{z})}. \quad (1.13)$$

If  $v \in \Delta_0$  then both functions  $Q_v^\infty(z)$  and  $Q_v(z)$  belong to the Nevanlinna class  $\mathcal{N}_0$ . The defect functions  $\varphi_v^\infty(\cdot, z)$  and  $\varphi_v(\cdot, z)$  are also well defined if  $v \in \Delta_1$ , however for  $z \in \mathbb{C}^+ \cup \mathbb{C}^-$  they do not belong to the space  $L^2(0, 1)$ . Moreover, the functions  $Q_v^\infty(z)$  and  $Q_v(z)$  exist for  $v \in \Delta_1$ , but one can show that they are no longer Nevanlinna functions but generalized Nevanlinna functions from the class  $\mathcal{N}_\kappa$  with  $\kappa = \left[\frac{v+1}{2}\right]$  and that the function  $Q_v^\infty(z)$  has a representation as  $N(z)$  in (1.6). According to what was said above, there are a Pontryagin space  $\Pi_\kappa$ , self-adjoint operators or relations  $H^\infty$  and  $H$ , a symmetric operator  $S = H^\infty \cap H$  in  $\Pi_\kappa$ , a Hilbert space  $\mathcal{H}_0$ , a self-adjoint operator  $A_0$  and a symmetric operator  $S_0$  in  $\mathcal{H}_0$ , such that

$$Q_v^\infty(z) \sim S, H^\infty \text{ in } \Pi_\kappa, \quad Q_v(z) \sim S, H \text{ in } \Pi_\kappa, \quad Q_0(z) \sim S_0, A_0 \text{ in } \mathcal{H}_0,$$

where  $Q_0(z)$  denotes the Nevanlinna function  $N_0(z)$  in representation (1.6) of  $Q_v^\infty(z)$ .

As mentioned above, if  $v \in \Delta_1$  the minimal operator  $L_v$  associated with the Bessel expression  $l_v$  is self-adjoint. We call in this case  $L_v$  the *Bessel operator*. There arises the problem to describe for  $v \in \Delta_1$  the spaces  $\Pi_\kappa$  and  $\mathcal{H}_0$ , the operators  $S, H, S_0, A_0$ , and the relation  $H^\infty$  in terms of the Bessel operator.

We mention two methods to construct these spaces and operators. Here we always suppose that  $v \in \Delta_1$  is fixed and often we do not write the index  $v$ .

In the *singular perturbation approach* we start from the triplet  $\{\mathcal{H}_0, A_0, \chi\}$ , where  $\mathcal{H}_0 = L^2(0, 1)$ ,  $A_0 = L_v$  is the Bessel operator in the Hilbert space  $L^2(0, 1)$  and  $\chi$  is the generalized element

$$\chi = (A_0 - z_0)\varphi^\infty(\cdot, z_0).$$

It will be shown in [7] that  $\chi \in \mathcal{H}_{-\kappa-1} \setminus \mathcal{H}_{-\kappa}$  (for the definition of these scale spaces associated with  $A_0$  we refer to Section 1.4 below) and that the function  $Q^\infty(z)$  admits the representation

$$Q^\infty(z) = c(z)^\kappa Q_0(z) + p(z),$$

where

$$Q_0(z) = a - i \operatorname{Im} Q_0(z_0) + (z - z_0^*) \langle (A_0 - z)^{-1} (A_0 - z_0)^{-\kappa} \chi, (A_0 - z_0)^{-\kappa-1} \chi \rangle_{L^2(0,1)}$$

with  $a \in \mathbb{R}$  such that  $\operatorname{Re} Q_0(i) = 0$  and  $p(z)$  is a real polynomial of degree at most  $2\kappa$ . The Pontryagin space  $\Pi_\kappa$  is obtained via a completion argument and turns out to

have the form

$$\Pi_\kappa = \mathcal{H}_0 \oplus (\mathcal{L} \dot{+} \mathcal{M}),$$

where  $\mathcal{L}$  is a  $\kappa$ -dimensional neutral subspace and  $\mathcal{M}$  is the span of the functions

$$u_j = \frac{1}{(j-1)!} \frac{d^{j-1}}{dz^{j-1}} \varphi^\infty(\cdot, z)|_{z=z_0} \in \mathcal{H}_{-\kappa-1+j} \setminus \mathcal{H}_{-\kappa+j}, \quad j = 1, 2, \dots, \kappa.$$

The self-adjoint relation  $H^\infty$  in  $\Pi_\kappa$ , which corresponds to the function  $Q^\infty(z)$ , is a ‘lifting’ of the self-adjoint operator  $A_0$  in  $\mathcal{H}_0$  to  $\Pi_\kappa$  such that  $\mathcal{L}$  is the root subspace of  $H^\infty$  at  $\infty$ , in fact  $\mathcal{H}_0$  is a Hilbert subspace of  $\Pi_\kappa$

$$P_0(H^\infty - z)^{-1}|_{\mathcal{H}_0} = (A_0 - z)^{-1},$$

where  $P_0$  is the projection in  $\Pi_\kappa$  onto  $\mathcal{H}_0$ , and hence

$$\sigma(Q^\infty) = \sigma(H^\infty) = \sigma(A_0) \cup \{\infty\}.$$

The operator  $H$  corresponding to  $Q(z) = -Q^\infty(z)^{-1}$  in (1.13) is defined via its resolvent

$$(H - z)^{-1} = (H^\infty - z)^{-1} - \frac{\langle \cdot, \varphi^\infty(\cdot, z^*) \rangle}{Q^\infty(z)} \varphi^\infty(\cdot, z).$$

In a more abstract setting this construction was developed by Shondin [25], van Diejen and Tip [6], and Dijkma et al. [10] in order to study the formal singular perturbation

$$A_0 + t^{-1} \langle \cdot, \chi \rangle_{L^2(0,1)} \chi, \quad t \in \mathbb{R}.$$

In the *infinite coupling approach* which we use in [7] we start with a triplet  $\{\Pi_\kappa, H, w\}$  constructed from the function  $\varphi(\cdot, z)$  in (1.12) and the function  $Q(z)$  in (1.13) as follows. The space  $\Pi_\kappa$  is the Pontryagin space generated by the sequence of functions  $\varphi^\infty(\cdot, \lambda_n)$ , where  $\varphi^\infty(\cdot, z) := -\frac{1}{Q(z)} \varphi(\cdot, z)$  and the  $\lambda_n$  are the poles of  $Q(z)$ , and equipped with the inner product inherited from the case  $0 < v < 1$  by analytic continuation arguments (cf. [13]) as explained, for example, in [11]. A self-adjoint operator  $H$  is defined in  $\Pi_\kappa$  by means of the relations

$$H\varphi^\infty(\cdot, \lambda_n) = \lambda_n \varphi^\infty(\cdot, \lambda_n);$$

thus the spectrum of  $H$  coincides with the set of poles of  $Q(z)$ . It will be shown in [7] that there exists an element  $w \in \text{dom } H^{\kappa-1} \setminus \text{dom } H^\kappa$  such that

$$\varphi(\cdot, z) = (H - z)^{-1}w,$$



the  $\kappa$ -dimensional subspace

$$\mathcal{L} := \text{span}\{w, Hw, \dots, H^{\kappa-1}w\}$$

is neutral,  $w$  is cyclic for  $H$  in  $\Pi_\kappa$ , and

$$Q(z) = \langle (H - z)^{-1}w, w \rangle, \quad z \in \rho(Q) = \rho(H).$$

We consider the one-parameter family of self-adjoint operators

$$H^{\langle \alpha \rangle} = H + \alpha \langle \cdot, w \rangle w, \quad \alpha \in \mathbb{R}.$$

If  $\alpha \rightarrow \infty$  the limit

$$\lim_{\alpha \rightarrow \infty} H^{\langle \alpha \rangle} =: H^\infty$$

exists in the strong resolvent sense and defines a self-adjoint relation  $H^\infty$ , such that  $Q_v^\infty(z) \sim S, H^\infty$  in  $\Pi_\kappa$  with  $S = H^\infty \cap H$ .

In an abstract Hilbert space situation Kiselev and Simon [16] termed  $H^\infty$  the *rank one perturbation of  $H$  and  $w$  with infinite coupling*; here we use their terminology (cf. also Gesztesy and Simon [14]). The infinite coupling approach was also used in connection with the Laguerre differential expression

$$l_v := -x \frac{d^2}{dx^2} - (1 + v - x) \frac{d}{dx} \quad \text{on } \mathbb{R}^+ = (0, \infty)$$

and the Hilbert space  $\mathcal{H}_0 = L^2(\mathbb{R}^+; w_v)$  with weight function  $w_v(x) = x^v e^{-x}$  in [3, 12]. In this paper the infinite coupling approach is developed in an abstract Pontryagin space setting.

**1.4.** We conclude the introduction with some notations, definitions and basic facts which will be used in the sequel. A function  $N(z)$  belongs to the class  $\mathcal{N}_0$  if and only if it admits an integral representation

$$N(z) = \alpha + \beta z + \int_{\mathbb{R}} \left( \frac{1}{t - z} - \frac{t}{t^2 + 1} \right) d\sigma(t), \quad (1.14)$$

where  $\alpha \in \mathbb{R}$ ,  $\beta \geq 0$  and  $\sigma(t)$  is a nondecreasing function on  $\mathbb{R}$  such that

$$\int_{\mathbb{R}} \frac{1}{t^2 + 1} d\sigma(t) < \infty.$$

We have

$$\alpha = \operatorname{Re} N(i), \quad \beta = \lim_{y \rightarrow \infty} \frac{1}{y} \operatorname{Im} N(iy) = \lim_{y \rightarrow \infty} \frac{1}{iy} N(iy),$$

and if  $\beta = 0$ , then

$$y \operatorname{Im} N(iy) = \int_{\mathbb{R}} \frac{y^2}{t^2 + y^2} d\sigma(t).$$

Thus (b) in (1.5) holds if and only if  $\beta = 0$ , and if this holds then (a) in (1.5) is equivalent to  $\int_{\mathbb{R}} d\sigma(t) = \infty$ .

The following proposition is a direct consequence of [18, Hauptsatz] and a remark on this paper. We give a more analytic proof and for this we use the following lemma proved in [15, Propositions 1.3 and 1.7].

**Lemma 1.1.** For  $N(z) \in \mathcal{N}_0$  and  $\widehat{N}(z) = -N(z)^{-1}$  we have

- (i)  $N(z) = \gamma + \int_{\mathbb{R}} \frac{d\sigma(t)}{t-z}$  with  $\int_{\mathbb{R}} d\sigma(t) < \infty \Leftrightarrow \sup_{y>0} y \operatorname{Im} N(iy) < \infty$ .
- (ii)  $\lim_{y \rightarrow \infty} y^{-1} \operatorname{Im} N(iy) > 0 \Leftrightarrow \lim_{y \rightarrow \infty} \widehat{N}(iy) = 0$  and  $\sup_{y>0} y \operatorname{Im} \widehat{N}(iy) < \infty$ .

**Proposition 1.2.** If  $N(z) \in \mathcal{N}_0$  then  $N(z)$  satisfies (1.5) if and only if  $\widehat{N}(z)$  satisfies (1.5).

**Proof.** It suffices to prove the “ $\Rightarrow$ ” part. Assume  $N(z)$  satisfies (1.5). The inequality

$$\frac{1}{y} |\widehat{N}(iy)| = \frac{1}{y|N(iy)|} \leq \frac{1}{y|\operatorname{Im} N(iy)|}, \quad y > 0,$$

and (1.5)(a) for  $N(z)$  implies (1.5)(b) for  $\widehat{N}(z)$ . We now prove that  $\widehat{N}(z)$  satisfies (a). Suppose the opposite holds:  $\sup_{y>0} y \operatorname{Im} \widehat{N}(iy) < \infty$ . Then by Lemma 1.1(i),

$$\widehat{N}(z) = \gamma + \int_{\mathbb{R}} \frac{d\sigma(t)}{t-z}, \quad \delta := \int_{\mathbb{R}} d\sigma(t) < \infty.$$

There are two possibilities:  $\gamma = 0$  and  $\gamma \neq 0$ . If  $\gamma = 0$ , then by Lemma 1.1(ii), we have  $\lim_{y \rightarrow \infty} y^{-1} \operatorname{Im} N(iy) > 0$  which contradicts (b) for  $N(z)$ . If  $\gamma \neq 0$ , then

$$N(z) = -\frac{1}{\gamma + \int_{\mathbb{R}} \frac{d\sigma(t)}{t-z}} \quad \text{and} \quad N(iy) = -\frac{1}{\gamma} + \frac{i\delta}{\gamma^2 y} + o\left(\frac{1}{y}\right), \quad y \rightarrow \infty.$$

Hence  $y \operatorname{Im} N(iy) = \frac{\delta}{\gamma^2} + o(1)$ . But this contradicts (a) for  $N(z)$ . Thus  $\widehat{N}(z)$  satisfies (a).  $\square$

If  $N(z) \in \mathcal{N}_\kappa$ , then  $z = \infty$  is the only pole of nonpositive type or generalized pole of nonpositive type if and only if  $N(z)$  admits integral representations of the form

$$N(z) = c(z)^m \int_{\mathbb{R}} \left( \frac{1}{t-z} - \frac{t}{t^2+1} \right) d\sigma(t) + p_\ell(z) \quad (1.15)$$

with  $c(z) = (z - z_0)(z - z_0^*)$ ,  $z_0 \in \mathbb{C} \setminus \mathbb{R}$ ,  $m \in \mathbb{N}_0$ , a nondecreasing function  $\sigma(t)$  on  $\mathbb{R}$  such that  $\int_{\mathbb{R}} (t^2 + 1)^{-1} d\sigma(t) < \infty$ , and a real polynomial  $p_\ell(z)$  of degree  $\ell$ . This follows from (1.6) and (1.4). As mentioned in Section 1.1 this representation can always be chosen irreducible which in terms of  $m$  and  $\sigma(t)$  means that either  $m = 0$ , or  $m > 0$  and  $\int_{\mathbb{R}} d\sigma(t) = \infty$ , and then the representation is unique. For the number  $\kappa$  of negative squares of  $N \in \mathcal{N}_\kappa$  with this irreducible representation the following formula holds, see [19, Lemma 3.3]; here  $a_\ell$  denotes the leading coefficient of the polynomial  $p_\ell(z)$ :

$$\kappa = \begin{cases} m & \text{if } \ell \leq 2m, \\ \frac{\ell + 1}{2} & \text{if } \ell > 2m, \ell \text{ is odd and } a_\ell < 0, \\ \left\lfloor \frac{\ell}{2} \right\rfloor & \text{otherwise.} \end{cases} \quad (1.16)$$

The functions  $N(z)$  in the class  $\mathcal{N}_\kappa^\infty$  are characterized as having an irreducible representation (1.15) in which  $\int_{\mathbb{R}} d\sigma(t) = \infty$  (even in the case  $m = 0$ ).

**Remark 1.3.** Assume  $N(z) \in \mathcal{N}_\kappa^\infty$  has the irreducible representation (1.15) and the irreducible representation

$$N(z) = c_1(z)^{m_1} \int_{\mathbb{R}} \left( \frac{1}{t - z} - \frac{t}{t^2 + 1} \right) d\sigma_1(t) + q(z)$$

with  $c_1(z) = (z - z_1)(z - z_1^*)$ ,  $z_1 \in \mathbb{C} \setminus \mathbb{R}$ ,  $m_1 \in \mathbb{N}_0$ , a nondecreasing function  $\sigma_1(t)$  on  $\mathbb{R}$  such that  $\int_{\mathbb{R}} (t^2 + 1)^{-1} d\sigma_1(t) < \infty$ , and a real polynomial  $q(z)$ . Then by the Stieltjes–Liřsic inversion formula we have  $c(t)^m d\sigma(t) = c_1(t)^{m_1} d\sigma_1(t)$ . Hence

$$\int_{\mathbb{R}} \frac{c(t)^m}{c_1(t)^{m_1}(t^2 + 1)} d\sigma(t) = \int_{\mathbb{R}} \frac{d\sigma_1(t)}{t^2 + 1} < \infty,$$

and this inequality and  $\int_{\mathbb{R}} d\sigma(t) = \infty$  imply  $m_1 \geq m$ . By the same reasoning  $m \geq m_1$ , and therefore  $m = m_1$ . Finally, the difference

$$p_\ell(z) - q(z) = \int_{\mathbb{R}} \frac{c_1(z)^m c(t)^m - c_1(t)^m c(z)^m}{t - z} \frac{(tz + 1)}{c(t)^m(t^2 + 1)} d\sigma(t)$$

is a polynomial of degree  $\leq 2m$ . Now it readily follows that the definition of the class  $\mathcal{N}_\kappa^\infty$  is independent of the choice of the reference point  $z_0 \in \mathbb{C} \setminus \mathbb{R}$ . Note that for a given  $N(z) \in \mathcal{N}_\kappa^\infty$  this point can actually be chosen from the larger set  $\rho(N)$ .

If  $A$  is a self-adjoint operator or a self-adjoint relation in some Pontryagin space  $\Pi_\kappa$ , the element  $w \in \Pi_\kappa$  is called *cyclic* for  $A$  if

$$\Pi_\kappa = \overline{\text{span}}\{w, (A - z)^{-1}w \mid z \in \rho(A)\},$$

or, equivalently, if for some (and then for every)  $z_0 \in \rho(A)$ , the function  $\varphi(z) = w + (z - z_0)(A - z)^{-1}w$  generates or spans the space  $\Pi_\kappa$ , that is,  $\Pi_\kappa = \overline{\text{span}}\{\varphi(z) \mid z \in \rho(A)\}$ . If  $A$  is an operator then  $w$  is cyclic for  $A$  if and only if

$$\Pi_\kappa = \overline{\text{span}}\{(A - z)^{-1}w \mid z \in \rho(A)\}.$$

With an unbounded self-adjoint operator  $A_0$  in the Hilbert space  $\mathcal{H}_0$  the scale of spaces  $\mathcal{H}_k$ ,  $k = \pm 1, \pm 2, \dots$ , is defined as follows. For positive index  $k$ ,  $\mathcal{H}_k$  is the linear space  $\text{dom } A_0^k$  equipped with the inner product and norm

$$\langle x, y \rangle_k := \sum_{j=0}^k \langle A_0^j x, A_0^j y \rangle_0, \quad \|x\|_k := \sqrt{\langle x, x \rangle_k}.$$

Denote by  $J_k$  the inclusion map  $\mathcal{H}_k \hookrightarrow \mathcal{H}_0$ . For  $f \in \mathcal{H}_0$ , the anti-linear mapping

$$x \in \mathcal{H}_k \mapsto \langle f, J_k x \rangle_0$$

is bounded on  $\mathcal{H}_k$ , and we set

$$\|f\|_{-k} := \sup \frac{\langle f, J_k x \rangle_0}{\|x\|_k}.$$

Then  $\|\cdot\|_{-k}$  defines a norm on  $\mathcal{H}_0$ , and the completion of  $\mathcal{H}_0$  with respect to this norm is the Hilbert space  $\mathcal{H}_{-k}$ . For further properties of these spaces see [1,10].

## 2. Rank one perturbation at infinite coupling

**2.1.** Let  $H$  be a self-adjoint operator in the Pontryagin space  $\Pi_\kappa$  and let  $w \in \Pi_\kappa$  be a cyclic element for  $H$ . For  $\alpha \in \mathbb{R}$  we consider the rank one perturbation  $H^{\langle \alpha \rangle}$  of  $H$  defined by

$$H^{\langle \alpha \rangle} := H + \alpha \langle \cdot, w \rangle w. \quad (2.1)$$

Evidently,  $H^{\langle \alpha \rangle}$  is a self-adjoint operator on  $\Pi_\kappa$ . With  $H^{\langle \alpha \rangle}$  and  $w$  we associate two functions defined on  $\rho(H^{\langle \alpha \rangle})$ : the function

$$\varphi^\alpha(z) = (H^{\langle \alpha \rangle} - z)^{-1}w, \quad z \in \rho(H^{\langle \alpha \rangle}),$$

which has values in  $\Pi_\kappa$ , and the scalar function

$$Q^\alpha(z) = \langle (H^{\langle \alpha \rangle} - z)^{-1}w, w \rangle, \quad z \in \rho(H^{\langle \alpha \rangle}).$$

Note that  $H^{\langle 0 \rangle} = H$ , and we shall write  $\varphi(z)$  for  $\varphi^0(z)$  and  $Q(z)$  for  $Q^0(z)$ :

$$\varphi(z) = (H - z)^{-1}w, \quad Q(z) = \langle (H - z)^{-1}w, w \rangle, \quad z \in \rho(H). \quad (2.2)$$

The operator  $S$ , defined in the following equivalent ways,

$$S := H|_{\{f \in \text{dom } H \mid \langle f, w \rangle = 0\}} = H \cap H^{\langle \alpha \rangle}, \quad \alpha \neq 0,$$

is a simple nondensely defined symmetric operator. The relation (here we use graph notation and  $\dot{+}$  stands for direct sum)

$$S^* = H \dot{+} \text{span}\{\{0, w\}\},$$

implies that  $S$  has defect index  $(1, 1)$ . Clearly,  $H^{\langle \alpha \rangle}$  is an extension of  $S$ . Its resolvent can be expressed in terms of the resolvent of  $H$ :

$$(H^{\langle \alpha \rangle} - z)^{-1} = (H - z)^{-1} - \frac{\langle \cdot, \varphi(z^*) \rangle}{Q(z) + \alpha^{-1}} \varphi(z), \quad z \in \rho(H) \cap \rho(H^{\langle \alpha \rangle}). \quad (2.3)$$

By definition,  $(H^{\langle \alpha \rangle} - z)\varphi^\alpha(z) = w$  and hence

$$\{\varphi^\alpha(z), 0\} = \{\varphi^\alpha(z), w\} + \{0, -w\} \in (H^{\langle \alpha \rangle} - z) \dot{+} \text{span}\{\{0, w\}\} = S^* - z,$$

which shows that  $\varphi^\alpha(z) \in \ker(S^* - z)$ . This together with the identity

$$\varphi^\alpha(z) - \varphi^\alpha(\zeta) = (z - \zeta)(H^{\langle \alpha \rangle} - z)^{-1} \varphi^\alpha(\zeta) \quad (2.4)$$

implies that  $\varphi^\alpha(z)$  is a defect function for  $S$  and  $H^{\langle \alpha \rangle}$ . Substitution of the right-hand side of (2.3) in the definitions of  $\varphi^\alpha(z)$  and  $Q^\alpha(z)$  yields the relations

$$\varphi^\alpha(z) = \frac{1}{1 + \alpha Q(z)} \varphi(z) \quad (2.5)$$

and

$$Q^\alpha(z) = \frac{Q(z)}{1 + \alpha Q(z)}. \quad (2.6)$$

The first of these and the fact that  $w$  is cyclic for  $H$  imply

$$\begin{aligned} \{\varphi^\alpha(z) \mid z \in \rho(H^{\langle \alpha \rangle})\} &= \overline{\text{span}}\{\varphi(z) \mid z \in \rho(H), \alpha Q(z) \neq -1\} \\ &= \overline{\text{span}}\{\varphi(z) \mid z \in \rho(H)\} = \Pi_\kappa, \end{aligned}$$

or, in words,  $w$  is cyclic for  $H^{\langle \alpha \rangle}$ . If in (2.4) we replace  $\zeta$  by  $\zeta^*$  and take the inner product of the expressions on both sides with  $w$ , we obtain

$$\frac{Q^\alpha(z) - Q^\alpha(\zeta)^*}{z - \zeta^*} = \langle \varphi^\alpha(z), \varphi^\alpha(\zeta) \rangle. \quad (2.7)$$

This shows that  $Q^\alpha(z)$  is a  $Q$ -function for  $S$  and  $H^{\langle \alpha \rangle}$ . Since the elements in the inner product on the right-hand side of this equality span the space  $\Pi_\kappa$  the equality also

shows that  $Q^\alpha \in \mathcal{N}_\kappa$ . The latter also follows from (2.6) since

$$\frac{Q^\alpha(z) - Q^\alpha(\zeta)^*}{z - \zeta^*} = \frac{1}{1 + \alpha Q(z)} \frac{Q(z) - Q(\zeta)^*}{z - \zeta^*} \frac{1}{1 + \alpha Q(\zeta)^*}.$$

Thus we have  $Q^\alpha \sim S, H^{\langle \alpha \rangle}$  in  $\Pi_\kappa$  and, on account of (2.6),

$$\rho(Q^\alpha) = \rho(H^{\langle \alpha \rangle}) = \{z \in \rho(H) \mid \alpha Q(z) \neq -1\}. \quad (2.8)$$

In these formulas the role of  $H$  can be taken over by any  $H^{\langle \beta \rangle}$ . Indeed, from (2.1) we get for  $\alpha, \beta \in \mathbb{R}$

$$H^{\langle \alpha \rangle} = H^{\langle \beta \rangle} + (\alpha - \beta) \langle \cdot, w \rangle w,$$

which yields for example the formula

$$\begin{aligned} (H^{\langle \alpha \rangle} - z)^{-1} &= (H^{\langle \beta \rangle} - z)^{-1} - \frac{\langle \cdot, \varphi^\beta(z^*) \rangle}{Q^\beta(z) + (\alpha - \beta)^{-1}} \varphi^\beta(z), \\ z \in \rho(H^{\langle \beta \rangle}) \cap \rho(H^{\langle \alpha \rangle}), \end{aligned} \quad (2.9)$$

and  $S = H^{\langle \alpha \rangle} \cap H^{\langle \beta \rangle}$ ,  $\alpha \neq \beta$ . Formulas (2.3) and (2.9) are Krein's parametrization formulas for the resolvents of all canonical self-adjoint extensions of  $S$ . They show that the family of all canonical self-adjoint extensions of  $S$  is given by  $\{H^{\langle \alpha \rangle}\}_{\alpha \in \mathbb{R} \cup \{\infty\}}$ , where  $H^{\langle \infty \rangle}$ , in the sequel denoted by  $H^\infty$ , is defined in the following theorem.

**Theorem 2.1.** *Let  $H$  be a self-adjoint operator in a Pontryagin space  $\Pi_\kappa$ , let  $w \in \Pi_\kappa$  be a cyclic element for  $H$ , and let  $S = H|_{\{f \in \text{dom } H \mid \langle f, w \rangle = 0\}}$ .*

(i) *For  $z \in \rho(H)$  with  $Q(z) \neq 0$  the limit*

$$R^\infty(z) := \lim_{|\alpha| \rightarrow \infty} (H^{\langle \alpha \rangle} - z)^{-1} \quad (2.10)$$

*exists with respect to the operator norm. It is the resolvent of a self-adjoint linear relation  $H^\infty$  with multi-valued part  $H^\infty(0) = \text{span}\{w\}$ . Moreover,  $\rho(H^\infty) \neq \emptyset$  and  $S = H \cap H^\infty$ .*

(ii) *For  $z \in \rho(H)$  and  $Q(z) \neq 0$  the limits*

$$\varphi^\infty(z) := \lim_{|\alpha| \rightarrow \infty} \alpha \varphi^\alpha(z), \quad Q^\infty(z) := \lim_{|\alpha| \rightarrow \infty} \alpha(\alpha Q^\alpha(z) - 1) \quad (2.11)$$

*exist and*

$$\varphi^\infty(z) = \frac{\varphi(z)}{Q(z)}, \quad Q^\infty(z) = -Q(z)^{-1}.$$

The function  $\varphi^\infty(z)$  is the defect function for  $S$  and  $H^\infty$ ,  $Q^\infty(z) \in \mathcal{N}_\kappa$ , and  $Q^\infty(z) \sim S, H^\infty$  in  $\Pi_\kappa$ , that is, with  $u = \varphi^\infty(z_0)$  for some  $z_0 \in \rho(H^\infty)$ ,

$$Q^\infty(z) = Q^\infty(z_0^*) + (z - z_0^*) \langle (I + (z - z_0)(H^\infty - z)^{-1})u, u \rangle, \quad z \in \rho(H^\infty),$$

and the minimality condition  $\Pi_\kappa = \overline{\text{span}} \{ \varphi^\infty(z) \mid z \in \rho(H^\infty) \}$  holds.

**Proof.** (i) If  $z \in \rho(H)$  and  $Q(z) \neq 0$ , then on account of (2.8) we have that  $z \in \rho(H^{\langle \alpha \rangle})$  for all  $\alpha$  with  $\alpha Q(z) \neq -1$ . This holds in particular if  $|\alpha| \rightarrow \infty$ . Formula (2.3) implies that the limit in (2.10) exists and equals

$$R^\infty(z) = R(z) - \frac{\langle \cdot, \varphi(z^*) \rangle}{Q(z)} \varphi(z), \quad R(z) := (H - z)^{-1}. \quad (2.12)$$

Consequently,  $R^\infty(z)$  is holomorphic on the set  $\rho(Q) \cap \rho(Q^{-1})$ , satisfies the resolvent identity, and the equality  $R^\infty(z)^* = R^\infty(z^*)$  holds. We have also

$$R^\infty(z)w = R(z)w - \frac{\langle w, \varphi(z^*) \rangle}{Q(z)} \varphi(z) = R(z)w - \varphi(z) = 0,$$

that is,  $\text{span}\{w\} \subset \ker R^\infty(z)$ . On account of  $\varphi(z) = R(z)w$  and (2.12) the inclusion is in fact an equality. Hence  $R^\infty(z) = (H^\infty - z)^{-1}$  is the resolvent of a self-adjoint linear relation  $H^\infty$  with a one-dimensional multi-valued part  $H^\infty(0) = \text{span}\{w\}$ . The resolvent set  $\rho(\mathcal{H}^\infty)$  is not empty because it contains  $\rho(Q) \cap \rho(Q^{-1})$ . For  $z \in \rho(H)$  and  $\alpha Q(z) \neq -1$ , we have  $(S - z)^{-1} \subset (H^{\langle \alpha \rangle} - z)^{-1}$  and hence  $(S - z)^{-1} \subset (H^\infty - z)^{-1}$ , that is,  $S \subset H^\infty$ . From  $S \subset H \cap H^\infty$  and  $\text{dom } H^\infty \perp w$  it follows that  $S = H \cap H^\infty$ .

(ii) For  $z \in \rho(H)$  with  $Q(z) \neq 0$  we have, by (2.5),

$$\varphi^\infty(z) := \lim_{|\alpha| \rightarrow \infty} \alpha \varphi^\alpha(z) = \frac{1}{Q(z)} \varphi(z),$$

where the limit is the strong limit in  $\Pi_\kappa$ , and by (2.6),

$$Q^\infty(z) := \lim_{|\alpha| \rightarrow \infty} \alpha(\alpha Q^\alpha(z) - 1) = -\frac{1}{Q(z)}.$$

Next we prove that  $\varphi^\infty(z)$  is a defect function for  $S$  and  $H^\infty$ . Indeed, as we have seen above,  $\varphi(z) \in \ker(S^* - z)$ ,  $z \in \rho(H)$ , and therefore if also  $Q(z) \neq 0$  then

$$\varphi^\infty(z) = \frac{1}{Q(z)} \varphi(z) \in \ker(S^* - z).$$

Multiplying (2.4) by  $\alpha$  and taking the limit as  $|\alpha| \rightarrow \infty$  we get the same equality for  $\alpha = \infty$ , which is just relation (1.1) for  $\varphi^\infty(z)$ . Hence  $\varphi^\infty(z)$  is a defect function for  $S$  and  $H^\infty$ . We have shown above that  $Q(z) \in \mathcal{N}_\kappa$ , but then  $Q^\infty(z) = -Q(z)^{-1} \in \mathcal{N}_\kappa$

also. Multiply both sides of equality (2.7) by  $\alpha^2$  and take the limit as  $|\alpha| \rightarrow \infty$ . Then for  $z, \zeta \in \rho(H)$  with  $Q(z) \neq 0$ ,  $Q(\zeta) \neq 0$ , we get the same equality but with  $\infty$  in place of  $\alpha$ :

$$\frac{Q^\infty(z) - Q^\infty(\zeta)^*}{z - \zeta^*} = \langle \varphi^\infty(z), \varphi^\infty(\zeta) \rangle$$

and this equality characterizes  $Q^\infty(z)$  as a  $Q$ -function of  $S$  and  $H^\infty$ . The minimality condition (1.4) holds for  $\varphi^\infty(z)$  because it holds for  $\varphi(z)$ . Hence  $Q^\infty \sim S, H^\infty$  in  $\Pi_\kappa$ .  $\square$

**Remark 2.2.** (a) Because of the minimality condition in Theorem 2.1(ii), we have

$$\rho(H^\infty) = \rho(Q^\infty) = \{z \in \rho(H) \mid Q(z) \neq 0\}.$$

(b) The following version of Krein's formula holds: For  $\alpha \in \mathbb{R}$ ,

$$(H^{\langle \alpha \rangle} - z)^{-1} = (H^\infty - z)^{-1} - \frac{\langle \cdot, \varphi^\infty(z^*) \rangle}{Q^\infty(z) - \alpha} \varphi^\infty(z), \quad z \in \rho(H^\infty) \cap \rho(H^{\langle \alpha \rangle}). \quad (2.13)$$

This follows from Theorem 2.1 and (2.9) by letting  $\beta \rightarrow \infty$ . If we multiply the numerator and denominator of the second summand on the right-hand side of (2.9) by  $\beta^2$ , then the denominator is transformed into

$$\beta^2(Q^\beta(z) + (\alpha - \beta)^{-1}) = \beta^2 Q^\beta(z) - \beta + \frac{\alpha\beta}{\alpha - \beta}$$

and has the limit  $Q^\infty(z) - \alpha$  as  $\beta \rightarrow \infty$ .

(c) The symmetric operator  $S$  can also be characterized by the equality

$$S = \{\{f, g\} \in H^\infty \mid \langle g - z^*f, \varphi^\infty(z) \rangle = 0\}.$$

The set on the right-hand side is independent of  $z \in \rho(H^\infty)$ .

(d) The element  $u = \varphi^\infty(z_0)$ ,  $z_0 \in \rho(H^\infty)$ , as in Theorem 2.1(ii), is cyclic but  $w$  is not cyclic for  $H^\infty$ , whereas if  $z_0 \in \rho(H^\infty) \cap \rho(H)$ , both  $u$  and  $w$  are cyclic for  $H$ . In fact, consider the function

$$\psi^\alpha(z) = u + (z - z_0)(H^{\langle \alpha \rangle} - z)^{-1}u$$

with values in  $\Pi_\kappa$ . Applying formula (2.13) we obtain the relation

$$\psi^\alpha(z) = -\frac{Q^\infty(z_0) - \alpha}{1 + \alpha Q(z)} \varphi(z) = -(Q^\infty(z_0) - \alpha) \varphi^\alpha(z).$$

Since  $w$  is cyclic for  $H^{\langle \alpha \rangle}$ ,  $\alpha \in \mathbb{R}$ , and  $u$  is cyclic for  $H^\infty$ , this relation implies that  $u$  is also cyclic for each  $H^{\langle \alpha \rangle}$ ,  $\alpha \in \mathbb{R} \cup \{\infty\}$ , except for  $\alpha = -Q(z_0)^{-1}$ .

(e) Finally, we note that if  $u = \varphi^\infty(z_0)$ ,  $z_0 \in \rho(H^\infty)$ , as in Theorem 2.1(ii), then  $\langle w, u \rangle = 1$ .



**2.2.** Let  $z_0 \in \rho(H^\infty)$ . If  $|\alpha|$  is sufficiently large then  $z_0 \in \rho(H^{\langle \alpha \rangle})$ , and for  $\alpha \rightarrow \infty$  the convergence of the operators  $(H^{\langle \alpha \rangle} - z_0)^{-1}$  to  $(H^\infty - z_0)^{-1}$  in the operator norm implies the convergence of the Cayley transforms  $U^\alpha := (H^{\langle \alpha \rangle} - z_0^*)(H^{\langle \alpha \rangle} - z_0)^{-1}$  of the operators  $H^{\langle \alpha \rangle}$  to the corresponding Cayley transform  $U^\infty$  of the relation  $H^\infty$  in (2.10) in the operator norm. Observing [18, Theorem 1.2] it follows that for  $\alpha \rightarrow \infty$  the eigenvalues of nonpositive type of  $U^\alpha$  converge to the eigenvalues of nonpositive type of  $U^\infty$ , and hence the eigenvalues of nonpositive type of  $H^{\langle \alpha \rangle}$  converge to the eigenvalues of nonpositive type of  $H^\infty$  in the closed convex plane. Denote the spectral functions (see, e.g., [17, 21]) of  $H^{\langle \alpha \rangle}$  and  $H^\infty$  by  $E^\alpha$  and  $E^\infty$ , respectively. An application of [24, Theorem 3.1] yields the following theorem.

**Theorem 2.3.** *Let  $H^{\langle \alpha \rangle}$  and  $H^\infty$  be as in Theorem 2.1. Then for each bounded interval  $\Delta$  of the real axis with endpoints not in  $\sigma_p(H^\infty)$  and which does not contain any eigenvalue of  $H^\infty$  of nonpositive type the relation*

$$\lim_{\alpha \rightarrow \infty} E^\alpha(\Delta) = E^\infty(\Delta)$$

*holds in the strong operator topology.*

For  $|\alpha|$  sufficiently large we consider the elements  $u^\alpha := \alpha \varphi^\alpha(z_0)$  and  $u = \varphi^\infty(z_0)$ . According to (2.11),  $u^\alpha \rightarrow u$  in  $\Pi_\kappa$  if  $\alpha \rightarrow \infty$ , and from Theorem 2.3 we conclude that

$$\lim_{\alpha \rightarrow \infty} \langle E^\alpha(\Delta) u^\alpha, u^\alpha \rangle = \langle E^\infty(\Delta) u, u \rangle \quad (2.14)$$

for each bounded interval  $\Delta$  of the real axis with endpoints not in  $\sigma_p(H^\infty)$ .

We denote by  $p_\alpha(z)$  the characteristic polynomial of the restriction of  $H^{\langle \alpha \rangle}$  to one of its maximal nonpositive invariant subspaces, and as in [24] we introduce the definitizing function  $r_\alpha(z)$  for  $H^{\langle \alpha \rangle}$  of the form

$$r_\alpha(z) = \frac{p_\alpha(z)p_\alpha^*(z)}{(z - z_0)^\kappa(z - z_0^*)^\kappa}.$$

Then it follows that

$$\langle (H^{\langle \alpha \rangle} - z)^{-1} w, w \rangle = r_\alpha(z)^{-1} \int \frac{d\sigma_\alpha(t)}{t - z} + r_\alpha(z)^{-1} \langle q_\alpha(z, H^{\langle \alpha \rangle}) w, w \rangle, \quad (2.15)$$

where  $q_\alpha(z, \zeta) := (z - \zeta)^{-1}(r_\alpha(z) - r_\alpha(\zeta))$  and  $\sigma_\alpha(t)$  is a bounded nondecreasing function on  $\mathbb{R}$ . Observing that  $u^\alpha = \alpha(H^{\langle \alpha \rangle} - z_0)^{-1} w$ , the inner product on the left-hand side of (2.14) can be written as

$$\langle E^\alpha(\Delta) u^\alpha, u^\alpha \rangle = \alpha^2 \int_\Delta \frac{d\sigma_\alpha(t)}{r_\alpha(t)(t - z_0)(t - z_0^*)}.$$

Relation (1.3) implies

$$(z - z_0)(z - z_0^*) \langle (H^\infty - z)^{-1} u, u \rangle = Q^\infty(z) - Q^\infty(z_0^*) - (z - z_0^*) \langle u, u \rangle,$$

and for the inner product on the right-hand side of (2.14) we obtain

$$\langle E^\infty(\Delta)u, u \rangle = -\frac{1}{2\pi i} \oint_{\Gamma_\Delta}' \frac{Q^\infty(z)}{(z - z_0)(z - z_0^*)} dz,$$

where  $\Gamma_\Delta$  is a closed contour which surrounds  $\Delta$ , does not surround  $z_0, z_0^*$  and intersects the real axis orthogonally at the endpoints of  $\Delta$ , and the prime at the integral denotes the Cauchy principal value. Thus (2.14) yields the relation

$$\lim_{\alpha \rightarrow \infty} \alpha^2 \int_\Delta \frac{d\sigma_\alpha(t)}{r_\alpha(t)(t - z_0)(t - z_0^*)} = -\frac{1}{2\pi i} \oint_{\Gamma_\Delta}' \frac{Q^\infty(z)}{(z - z_0)(z - z_0^*)} dz. \quad (2.16)$$

This formula will be specified further in Section 5, see Remark 5.3.

### 3. Generalized Nevanlinna functions with a pole or generalized pole of nonpositive type at $\infty$

The infinite coupling method associated with a self-adjoint operator  $H$  in a Pontryagin space  $\Pi_\kappa$  and a cyclic element  $w$  for  $H$  in the previous section leads to two generalized Nevanlinna functions  $Q(z) = \langle (H - z)^{-1}w, w \rangle$  and  $Q^\infty(z)$  related by the formula  $Q^\infty(z) = -Q(z)^{-1}$ . In this section we study the connection between the operator representations of a function  $N(z) \in \mathcal{N}_\kappa$  and the function  $-N(z)^{-1}$  directly. As an example we mention the functions  $Q_v(z)$  and  $Q_v^\infty(z)$  related to the Bessel operator (see Section 1.2).

**Theorem 3.1.** *For the generalized Nevanlinna functions  $N(z) \in \mathcal{N}_\kappa$  and  $\widehat{N}(z) = -N(z)^{-1}$  the following statements are equivalent:*

(i)  $N(z)$  has a representation

$$N(z) = \langle (A - z)^{-1}w, w \rangle, \quad z \in \rho(N), \quad (3.1)$$

where  $A$  is a self-adjoint operator in a Pontryagin space  $\Pi_\kappa$  and  $w \in \Pi_\kappa$  is a cyclic element for  $A$ .

(ii)  $\widehat{N}(z)$  has a representation

$$\widehat{N}(z) = \widehat{N}(z_0^*) + (z - z_0^*) \langle (I + (z - z_0)(\widehat{A} - z)^{-1})u, u \rangle, \quad z \in \rho(\widehat{N}), \quad (3.2)$$

where  $z_0 \in \rho(\widehat{N})$ ,  $\widehat{A}$  is a self-adjoint linear relation in a Pontryagin space  $\widehat{\Pi}_\kappa$  with nontrivial multi-valued part  $\widehat{A}(0)$  and nonempty resolvent set  $\rho(\widehat{A})$ , and  $u \in \widehat{\Pi}_\kappa$  is a cyclic element for  $\widehat{A}$ .

Representations (3.1) and (3.2) can be chosen such that (a) the Pontryagin spaces  $\Pi_\kappa$  and  $\widehat{\Pi}_\kappa$  coincide, (b)  $w \in \widehat{A}(0)$  and  $\langle u, w \rangle = 1$ , (c) the symmetric operator  $S := A \cap \widehat{A}$  has defect index  $(1, 1)$  and (d)  $N \sim S, A$  and  $\widehat{N} \sim S, \widehat{A}$  in  $\Pi_\kappa$ .

**Remark 3.2.** In the proof of Theorem 3.1 the following relations between  $A, \widehat{A}, w$ , and  $u$  will be established:

$$(\widehat{A} - z)^{-1} = (A - z)^{-1} - \frac{\langle \cdot, \varphi(z^*) \rangle}{N(z)} \varphi(z), \quad \varphi(z) := (A - z)^{-1} w, \quad (3.3)$$

$$(A - z)^{-1} = (\widehat{A} - z)^{-1} - \frac{\langle \cdot, \widehat{\varphi}(z^*) \rangle}{\widehat{N}(z)} \widehat{\varphi}(z), \quad \widehat{\varphi}(z) := u + (z - z_0)(A - z)^{-1} u, \quad (3.4)$$

and

$$\widehat{\varphi}(z) = \frac{1}{N(z)} \varphi(z), \quad u = \frac{1}{N(z_0)} \varphi(z_0). \quad (3.5)$$

Moreover,  $\varphi(z)$  is a defect function associated with  $S$  and  $A$  and  $\widehat{\varphi}(z)$  is a defect function associated with  $S$  and  $\widehat{A}$ .

Note that (3.3) implies

$$\text{dom } \widehat{A} \subset \text{dom } A \quad (3.6)$$

and  $\text{dom } \widehat{A} \neq \text{dom } A$  because  $A$  is densely defined, whereas  $\widehat{A}$  is not. In combination with (3.4) we find that for any  $z \in \rho(A) \cap \rho(\widehat{A})$ ,

$$\text{dom } A = \text{dom } \widehat{A} \dot{+} \text{span}\{\varphi(z)\}.$$

**Proof of Theorem 3.1.** (i)  $\Rightarrow$  (ii) Assume  $N(z)$  has representation (i). Define  $\varphi(z)$  as in (3.3), set  $R(z) = (A - z)^{-1}$ , and denote the right-hand side of the first relation in (3.3) by  $\widehat{R}(z)$ . From  $R(z)^* = R(z^*)$ ,

$$R(z) - R(\zeta) = (z - \zeta)R(z)R(\zeta), \quad (3.7)$$

and

$$\frac{N(z) - N(\zeta)}{z - \zeta} = \langle \varphi(z), \varphi(\zeta^*) \rangle, \quad (3.8)$$

we obtain after some calculations that  $\widehat{R}(z)^* = \widehat{R}(z^*)$  and

$$\widehat{R}(z) - \widehat{R}(\zeta) = (z - \zeta)\widehat{R}(z)\widehat{R}(\zeta).$$

These equalities imply that  $\widehat{R}(z)$  is the resolvent of some self-adjoint relation  $\widehat{A}$  in  $\Pi_\kappa$  with a nonempty resolvent set  $\rho(\widehat{A})$ :

$$\widehat{A} = \{ \{ \widehat{R}(z)h, h + z\widehat{R}(z)h \} \mid h \in \Pi_\kappa \}, \quad z \in \rho(\widehat{A}),$$

where the set on the right-hand side is independent of  $z \in \rho(\widehat{A})$ . Having defined  $\widehat{A}$  this way, we shall prove later that  $\widehat{A}$  can be taken as the self-adjoint relation in the representation of  $\widehat{N}(z)$  in part (ii). First we prove the other formulas in Remark 3.2. From (3.3) it readily follows that  $\widehat{R}(z)w = 0$ ,  $z \in \rho(\widehat{A})$ , and hence  $w \in \widehat{A}(0)$ . Define  $\widehat{\varphi}(z)$  as in (3.5). Then the first relation in (3.4) follows from (3.3) via a simple substitution. From (3.3), (3.7), and (3.8) we get

$$\begin{aligned} & (1 + (z - \zeta)(\widehat{A} - z)^{-1})\varphi(\zeta) \\ &= \varphi(\zeta) + (z - \zeta)(A - z)^{-1}\varphi(\zeta) - (z - \zeta) \frac{\langle \varphi(\zeta), \varphi(z^*) \rangle}{N(z)} \varphi(z) \\ &= \varphi(\zeta) + (\varphi(z) - \varphi(\zeta)) - \frac{N(z) - N(\zeta)}{N(z)} \varphi(z) = \frac{N(\zeta)}{N(z)} \varphi(z), \end{aligned}$$

and hence

$$\widehat{\varphi}(z) = (1 + (z - \zeta)(\widehat{A} - z)^{-1})\widehat{\varphi}(\zeta) = (1 + (z - z_0)(\widehat{A} - z)^{-1})u, \quad u := \widehat{\varphi}(z_0).$$

This proves that  $\widehat{\varphi}(z)$  can be represented as in (3.4) and the formula for  $u$  in (3.5). Finally, by (3.1), (3.5), and the second relation in (3.3):

$$\langle u, w \rangle = \frac{1}{N(z_0)} \langle (A - z_0)^{-1}w, w \rangle = 1. \quad (3.9)$$

The representation formula for  $\widehat{N}(z)$  in part (i) follows from

$$(z - z_0) \langle \widehat{\varphi}(z), u \rangle = (z - z_0) \frac{\langle \varphi(z), \varphi(z_0) \rangle}{N(z)N(z_0)^*} = N(z) - N(z_0)^*,$$

where for the last equality we used (3.8). Thus (ii) implies (i) and also the relations in Remark 3.2 hold.

(ii)  $\Rightarrow$  (i) If  $\widehat{N}(z)$  is as in (ii) define  $\widehat{\varphi}(z)$  by the second relation in (3.4). Let  $w \in \widehat{A}(0)$  and  $w \neq 0$ . Then  $\langle u, w \rangle \neq 0$ : Otherwise

$$\langle \widehat{\varphi}(z), w \rangle = \langle u, w \rangle + (z - z_0) \langle u, (\widehat{A} - z^*)^{-1}w \rangle = 0,$$

and, since  $u$  is cyclic for  $\widehat{A}$ , we see that  $w = 0$ . Thus we can choose  $w \in \widehat{A}(0)$  such that  $\langle u, w \rangle = 1$ . From the definition of  $\widehat{\varphi}(z)$  we obtain

$$\frac{\widehat{N}(z) - \widehat{N}(\zeta)}{z - \zeta} = \langle \widehat{\varphi}(z), \widehat{\varphi}(\zeta^*) \rangle$$

and

$$(A - z)^{-1} \widehat{\varphi}(\zeta) = \frac{\widehat{\varphi}(z) - \widehat{\varphi}(\zeta)}{z - \zeta}.$$

With the help of these formulas one can show that the right-hand side of the first equality in (3.4) is the resolvent of a self-adjoint relation which we denote by  $A$ , and thus (3.4) holds. By (3.4) and (3.9),

$$\varphi(z) = -\frac{\langle w, \widehat{\varphi}(z^*) \rangle}{\widehat{N}(z)} \widehat{\varphi}(z) = -\frac{\langle w, u \rangle}{\widehat{N}(z)} \widehat{\varphi}(z) = N(z) \widehat{\varphi}(z),$$

that is, (3.5) is valid. We claim that  $A$  is an operator. To see this, let  $x \in A(0)$ . Then  $(A - z)^{-1}x = 0$  and, since  $w \in \widehat{A}(0)$ , by (3.4) and (3.9), for all  $z \in \rho(\widehat{A})$  with  $\widehat{N}(z) \neq 0$ ,

$$0 = \langle (A - z)^{-1}x, w \rangle = \frac{\langle x, \widehat{\varphi}(z^*) \rangle}{\widehat{N}(z)}.$$

This implies that  $x = 0$ , proving the claim. Finally, (3.4) and (3.5) imply (3.3), and (3.3) in turn yields (3.2). Thus we have shown the implication (ii)  $\Rightarrow$  (i).

The proofs of the remaining statements in the theorem are left to the reader. We only remark that the symmetric operator  $S$  can be defined by

$$S = \{\{f, h\} \in \widehat{A} \mid \langle h - z^*f, \varphi(z) \rangle = 0\} = \{\{f, h\} \in A \mid \langle h - z^*f, \varphi(z) \rangle = 0\}.$$

Here the set in the middle is independent of  $z \in \rho(\widehat{A})$  because

$$\{\widehat{\varphi}(z), z\widehat{\varphi}(z)\} - \{u, z_0u\} \in A. \quad \square$$

#### 4. Generalized Nevanlinna functions in the class $\mathcal{N}_\kappa^\infty$

**Lemma 4.1.** *Let  $A$  be a densely defined self-adjoint operator in a Pontryagin space  $\Pi_\kappa$ , and  $w \in \Pi_\kappa$ ,  $w \neq 0$ . Equivalent are:*

(a) *The function  $\langle (A - z)^{-1}w, w \rangle$  admits a representation*

$$\langle (A - z)^{-1}w, w \rangle = -\sum_{j=1}^{2n-1} \frac{s_{j-1}}{z^j} + \frac{M(z)}{z^{2n-1}}$$

*with a function  $M(z)$  having the properties*

$$M(iy) \rightarrow 0, \quad y^2 \operatorname{Re} M(iy) \rightarrow +\infty \quad \text{if } y \uparrow +\infty. \quad (4.1)$$

(b)  $w \in \operatorname{dom} A^{n-1} \setminus \operatorname{dom} A^n$ .

**Proof.** If (b) holds then

$$\langle (A - z)^{-1}w, w \rangle = - \sum_{j=1}^n \frac{\langle A^{j-1}w, w \rangle}{z^j} - \sum_{j=n+1}^{2n-1} \frac{\langle A^{n-1}w, A^{j-n}w \rangle}{z^j} + \frac{M(z)}{z^{2n-1}}$$

with

$$M(z) = \langle A(A - z)^{-1}A^{n-1}w, A^{n-1}w \rangle.$$

Observe that

$$\begin{aligned} \operatorname{Re} M(z) &= \langle A(A - z)^{-1}A^{n-1}w, A(A - z)^{-1}A^{n-1}w \rangle \\ &\quad - (\operatorname{Re} z) \langle A(A - z)^{-1}A^{n-1}w, A^{n-1}w \rangle. \end{aligned}$$

Using the spectral function  $E$  of  $A$  (see [17,21]),  $M(z)$  can be written as

$$M(z) = M_0(z) + \int_{|t| \geq \gamma} \frac{t}{t - z} d\sigma(t)$$

with  $\gamma > 0$ , sufficiently large,  $d\sigma(t) = \langle E(dt)A^{n-1}w, A^{n-1}w \rangle$ , and a function  $M_0(z)$  which is holomorphic at  $\infty$  and has the properties

$$M_0(z) = O\left(\frac{1}{|z|}\right), \quad |z| \rightarrow \infty, \quad \operatorname{Re} M_0(iy) = O\left(\frac{1}{y^2}\right), \quad y \rightarrow \infty.$$

Now the first relation in (4.1) is clear, the second relation follows from

$$y^2 \operatorname{Re} M(iy) = y^2 \int_{|t| \geq \gamma} \frac{t^2}{t^2 + y^2} d\sigma(t) + o(1) \rightarrow +\infty, \quad y \uparrow \infty, \quad (4.2)$$

since  $\int_{|t| \geq \gamma} t^2 d\sigma(t) = \infty$ , which is a consequence of  $A^{n-1}w \notin \operatorname{dom} A$ .

Conversely, if (a) holds then, according to [19, Satz 1.10],  $w \in \operatorname{dom} A^{n-1}$ , and, as in (4.2),  $w \in \operatorname{dom} A^n$  would yield  $\lim_{y \rightarrow \infty} y^2 \operatorname{Re} M(iy) < \infty$ , contradicting (4.1).  $\square$

In the following, for  $m = 0$  the subspace  $\operatorname{span}\{w, Aw, \dots, A^{m-1}w\}$  consists only of the zero element, and for  $q = 0$  the sum  $\sum_{j=2m}^{2m+q-1}$  is zero, etc.

**Theorem 4.2.** For the functions  $N(z)$  and  $\widehat{N}(z) = -N(z)^{-1}$ , the following assertions are equivalent:

(i)  $N(z)$  has a representation (3.1):

$$N(z) = \langle (A - z)^{-1}w, w \rangle, \quad z \in \rho(N),$$

where  $A$  is a self-adjoint operator in a Pontryagin space  $\Pi_\kappa$ ,  $w \in \Pi_\kappa$  is a cyclic element for  $A$  with the property

$$w \in \operatorname{dom} A^{m+q-1} \setminus \operatorname{dom} A^{m+q}$$

for some integers  $m, q \in \mathbb{N}_0, m+q > 0$ , the subspace

$$\mathcal{L} := \operatorname{span}\{w, Aw, \dots, A^{m-1}w, A^m w, \dots, A^{m+q-1}w\}$$

has index of nonpositivity  $\kappa$ , and

$$\begin{aligned} \langle A^j w, A^k w \rangle &= 0, \quad 0 \leq j, \quad k \leq m+q-1, \quad j+k \leq 2m+q-2, \\ \langle A^j w, A^k w \rangle &\neq 0, \quad 0 \leq j, \quad k \leq m+q-1, \quad j+k = 2m+q-1. \end{aligned} \quad (4.3)$$

(ii)  $N(z) \in \mathcal{N}_\kappa$ ,  $z = \infty$  is the only zero of nonpositive type or generalized zero of nonpositive type of  $N(z)$ , and  $N(z)$  has a representation

$$N(z) = - \sum_{j=2m+q}^{2m+2q-1} \frac{s_{j-1}}{z^j} + \frac{1}{z^{2m+2q-1}} M(z), \quad (4.4)$$

with  $m, q \in \mathbb{N}_0, m+q > 0$ , real numbers  $s_j, j = 2m+q-1, \dots, 2m+2q-2$ ,  $s_{2m+q-1} \neq 0$  if  $q > 0$ , and a function  $M(z)$  with the properties

$$\lim_{y \rightarrow \infty} M(iy) = 0, \quad \lim_{y \rightarrow \infty} y^2 \operatorname{Re} M(iy) = +\infty. \quad (4.5)$$

(iii)  $\widehat{N}(z)$  has a representation (3.2):

$$\widehat{N}(z) = \widehat{N}(z_0^*) + (z - z_0^*) \langle (I + (z - z_0)(\widehat{A} - z)^{-1})u, u \rangle, \quad z \in \rho(\widehat{N}),$$

where  $z_0 \in \rho(\widehat{N})$ ,  $\widehat{A}$  is a self-adjoint linear relation in a Pontryagin space  $\widehat{\Pi}_\kappa$ ,  $\rho(\widehat{A}) \neq \emptyset$ ,  $u \in \widehat{\Pi}_\kappa$  is a cyclic element for  $\widehat{A}$ , the root space  $\widehat{\mathcal{L}}$  of  $\widehat{A}$  at  $z = \infty$  is spanned by  $m+q$  vectors  $w_1, w_2, \dots, w_{m+q}$ , which form a Jordan chain of  $\widehat{A}$  at  $\infty$ ,  $\widehat{\mathcal{L}}$  has index of nonpositivity  $\kappa$  and  $\operatorname{span}\{w_1, w_2, \dots, w_m\}$  is its isotropic subspace. If  $m = 0$  and  $P_0$  denotes the orthogonal projection onto  $\mathcal{H}_0 := \widehat{\Pi}_\kappa \ominus \widehat{\mathcal{L}}$ , which is a uniformly positive subspace of  $\widehat{\Pi}_\kappa$ , then  $P_0 u \notin \operatorname{dom} \widehat{A}$ .

(iv)  $\widehat{N}(z) \in \mathcal{N}_\kappa^\infty$ , the irreducible representation of  $\widehat{N}(z)$  being

$$\widehat{N}(z) = c(z)^m \widehat{N}_0(z) + p_\ell(z), \quad c(z) = (z - z_0)(z - z_0^*),$$

where  $z_0 \in \mathbb{C} \setminus \mathbb{R}$ ,  $m \in \mathbb{N}_0$ ,  $p_\ell(z) = \sum_{k=0}^{\ell} a_k z^k$  is a real polynomial of degree  $\ell$ ,  $\widehat{N}_0(z) \in \mathcal{N}_0$  has properties (1.7):

$$\lim_{y \rightarrow +\infty} y \operatorname{Im} \widehat{N}_0(iy) = +\infty, \quad \lim_{y \rightarrow \infty} y^{-1} \widehat{N}_0(iy) = 0, \quad \operatorname{Re} \widehat{N}_0(i) = 0,$$

and we set  $q := \max\{\ell - 2m, 0\}$ .

The Pontryagin spaces in (i) and (iii) can be chosen the same and then the element  $w_1$  in (iii) can be chosen to coincide with  $w$  in (i) and to satisfy  $\langle w_1, u \rangle = 1$ ; in this case  $w_j = A^{j-1}w$ ,  $j = 1, \dots, m+q$ , and  $\mathcal{L} = \widehat{\mathcal{L}}$ . With  $A$  and  $w$  from (i) and the coefficients  $s_j$ ,  $2m+q-1 \leq j \leq 2m+2q-2$  in (4.4),  $s_j = 0$  if  $0 \leq j \leq 2m+q-2$ , it holds

$$s_j = \langle A^r w, A^s w \rangle \quad \text{if } r+s=j, \quad 0 \leq r, \quad s \leq m+q-1, \quad (4.6)$$

and  $s_{2m+q-1} = \frac{1}{a_{2m+q}} = \frac{1}{a_\ell}$  if  $q > 0$ . The relation between the integers  $\kappa, m$ , and  $q$  is

$$\kappa = \begin{cases} m & \text{if } q = 0, \\ m + \frac{q+1}{2} & \text{if } q > 0, \quad q \text{ odd}, \quad a_\ell < 0, \\ m + \left\lfloor \frac{q}{2} \right\rfloor & \text{otherwise.} \end{cases} \quad (4.7)$$

**Remark 4.3.** (1) Observe that in (i) in the case  $m > 0$  relations (4.3) are equivalent to the fact that  $\operatorname{span}\{w, Aw, \dots, A^{m-1}w\}$  is the isotropic subspace of  $\mathcal{L}$ .

(2) The elements  $w_1, w_2, \dots, w_{m+q}$  form a Jordan chain of  $\widehat{A}$  at  $\infty$  (see (iii)) if and only if for some (and then for every)  $z \in \rho(\widehat{A})$  we have

$$\begin{aligned} (\widehat{A} - z)^{-1} w_1 &= 0, \\ (\widehat{A} - z)^{-1} w_j &= w_{j-1} + z w_{j-2} + \dots + z^{j-2} w_1, \quad j = 2, 3, \dots, m+q. \end{aligned} \quad (4.8)$$

**Proof of Theorem 4.2.** We show the implications

$$(iv) \Rightarrow (ii) \Rightarrow (i) \Rightarrow (iii) \Rightarrow (iv).$$

(iv)  $\Rightarrow$  (ii): Because of Remark 1.3, without loss of generality we may assume  $z_0 = i$ . First we suppose that  $\ell \leq 2m$ . Then, if we set  $a_{2m} = 0$  for  $\ell < 2m$ ,

$$N(z) = -\frac{1}{(1+z^2)^m \widehat{N}_0(z) + a_{2m} z^{2m} + 0(z^{2m-1})} = -\frac{1}{z^{2m-1}} M(z)$$



with

$$M(z) = -\frac{1}{z(\alpha(z)\widehat{N}_0(z) + a_{2m} + \frac{0(1)}{z})}, \quad \alpha(z) := \frac{(1+z^2)^m}{z^{2m}},$$

hence

$$M(iy) = -\frac{1}{iy(\widehat{N}_0(iy) + a_{2m}) + iy(\alpha(iy) - 1)\widehat{N}_0(iy) + 0(1)}.$$

The function  $\widetilde{N}_0(z) := \widehat{N}_0(z) + a_{2m}$ , like  $\widehat{N}(z)$ , also has properties (1.5), therefore the first summand in the denominator tends to  $\infty$ , the second one tends to zero and the third one remains bounded. It follows that

$$|M(iy)| \rightarrow 0 \quad \text{if } y \rightarrow \infty.$$

Further, observing that  $\alpha(iy) = \frac{(y^2-1)^m}{y^{2m}}$ , for  $y \rightarrow \infty$  we obtain

$$\begin{aligned} y^2 \operatorname{Re} M(iy) &= -y \operatorname{Im} \frac{1}{\left(\alpha(iy)\widehat{N}_0(iy) + a_{2m} + \frac{0(1)}{y}\right)} \\ &= y \frac{\alpha(iy) \operatorname{Im} \widetilde{N}_0(iy) + \frac{0(1)}{y}}{|\alpha(iy)\widetilde{N}_0(iy) + a_{2m}(1 - \alpha(iy)) + \frac{0(1)}{y}|^2} \\ &= \frac{1}{\alpha(iy)|\widetilde{N}_0(iy)|^2} \frac{y \operatorname{Im} \widetilde{N}_0(iy) + 0(1)}{|1 + a_{2m} \frac{1 - \alpha(iy)}{\alpha(iy)\widetilde{N}_0(iy)} + \frac{0(1)}{y\widetilde{N}_0(iy)}|^2}, \end{aligned}$$

which, for  $y$  large enough, is larger than

$$\frac{1}{2} \frac{1}{\alpha(iy)} \frac{1}{|1 + a_{2m} \frac{1 - \alpha(iy)}{\alpha(iy)\widetilde{N}_0(iy)} + \frac{0(1)}{y\widetilde{N}_0(iy)}|^2} \frac{y \operatorname{Im} \widetilde{N}_0(iy)}{|\widetilde{N}_0(iy)|^2}.$$

It remains to observe that the last factor equals  $-y \operatorname{Im} \frac{1}{\widetilde{N}_0(iy)}$  and that with  $\widehat{N}_0(z)$  also  $\widetilde{N}_0(z)$  and, by Proposition 1.2,  $-\frac{1}{\widetilde{N}_0(z)}$  have properties (1.5).

If  $\ell > 2m$  then with  $\widetilde{p}_\ell(z) := \frac{p_\ell(z)}{z^\ell}$ :

$$\begin{aligned} N(z) &= -\frac{1}{p_\ell(z) + (1+z^2)^m \widehat{N}_0(z)} \\ &= -\frac{1}{p_\ell(z)} + \frac{(1+z^2)^m \widehat{N}_0(z)}{p_\ell(z)(p_\ell(z) + (1+z^2)^m \widehat{N}_0(z))} \\ &= -\frac{1}{z^\ell \widetilde{p}_\ell(z)} + \frac{\alpha(z)\widehat{N}_0(z)}{z^{2\ell-2m} \widetilde{p}_\ell(z) \left( \widetilde{p}_\ell(z) + \frac{(1+z^2)^m}{z^\ell} \widehat{N}_0(z) \right)}. \end{aligned}$$

Further, there exist real numbers  $s_j$ , such that for  $|z| \rightarrow \infty$

$$-\frac{1}{z^\ell \tilde{\mathbf{p}}_\ell(z)} = -\sum_{j=\ell}^{\ell+q-1} \frac{s_{j-1}}{z^j} - \frac{s_{\ell+q-1}}{z^{\ell+q}} + \frac{1}{z^{\ell+q}} o\left(\frac{1}{z}\right).$$

It follows that

$$\begin{aligned} N(z) &= -\sum_{j=\ell}^{\ell+q-1} \frac{s_{j-1}}{z^j} - \frac{s_{\ell+q-1}}{z^{\ell+q}} + \frac{1}{z^{\ell+q}} o\left(\frac{1}{z}\right) + \frac{\alpha(z) \widehat{N}_0(z)}{z^{\ell+q} \tilde{\mathbf{p}}_\ell(z) (\tilde{\mathbf{p}}_\ell(z) + \frac{(1+z^2)^m}{z^\ell} \widehat{N}_0(z))} \\ &= -\sum_{j=\ell}^{\ell+q-1} \frac{s_{j-1}}{z^j} + \frac{1}{z^{\ell+q-1}} M(z) \end{aligned}$$

with

$$M(z) := -\frac{s_{\ell+q-1}}{z} + o\left(\frac{1}{z^2}\right) + \frac{\alpha(z) \widehat{N}_0(z)}{z \tilde{\mathbf{p}}_\ell(z) (\tilde{\mathbf{p}}_\ell(z) + \frac{(1+z^2)^m}{z^\ell} \widehat{N}_0(z))}, \quad |z| \rightarrow \infty.$$

Using again relations (1.5), we obtain for  $y \rightarrow \infty$ :  $M(iy) \rightarrow 0$  and

$$\begin{aligned} \operatorname{Re} M(iy) &= o\left(\frac{1}{y^2}\right) + \operatorname{Re} \frac{\alpha(iy) \widehat{N}_0(iy)}{iy \tilde{\mathbf{p}}_\ell(iy) (\tilde{\mathbf{p}}_\ell(iy) + \frac{(1-y^2)^m}{(iy)^\ell} \widehat{N}_0(iy))} \\ &= o\left(\frac{1}{y^2}\right) + \operatorname{Im} \frac{\alpha(iy) \widehat{N}_0(iy)}{y \tilde{\mathbf{p}}_\ell(iy) (\tilde{\mathbf{p}}_\ell(iy) + \frac{(1-y^2)^m}{(iy)^\ell} \widehat{N}_0(iy))} \\ &= o\left(\frac{1}{y^2}\right) + \operatorname{Im} \frac{\alpha(iy) \widehat{N}_0(iy)}{ya_\ell^2 + o(1) + \frac{a_\ell(1-y^2)^m}{i(iy)^{\ell-1}} \widehat{N}_0(iy) + o(1)}, \end{aligned}$$

$$y^2 \operatorname{Re} M(iy) = o(1) + \operatorname{Im} \frac{\alpha(iy) \widehat{N}_0(iy)}{\frac{a_\ell^2}{y} + o(\frac{1}{y^2}) + \frac{a_\ell(1-y^2)^m}{i(iy)^{\ell-1} y^2} \widehat{N}_0(iy) + o(\frac{1}{y^2})}.$$

If we divide the numerator and the denominator by  $N_0(iy)$ , then all the four terms in the denominator tend to zero as  $y \rightarrow \infty$  and, finally,

$$\lim_{y \rightarrow +\infty} y^2 \operatorname{Re} M(iy) = +\infty.$$

(ii)  $\Rightarrow$  (i) is a consequence of Lemma 4.1 and of relation (4.6).

(i)  $\Rightarrow$  (iii): First we show that for the elements  $w_j = A^{j-1}w$ ,  $j = 1, \dots, m+q$ , relations (4.8) hold. To this end we observe relations (3.3) and (3.1)

and obtain

$$(\widehat{A} - z)^{-1}w_1 = (A - z)^{-1}w - \frac{\langle (A - z)^{-1}w, w \rangle}{N(z)}(A - z)^{-1}w = 0,$$

and for  $2 \leq j \leq m + q$ , using that

$$(A - z)^{-1}A^{j-1} = z^{j-1}(A - z)^{-1} + \sum_{k=0}^{j-2} z^k A^{j-k-2},$$

in an analogous way

$$\begin{aligned} (\widehat{A} - z)^{-1}w_j &= (A - z)^{-1}A^{j-1}w - \frac{\langle (A - z)^{-1}A^{j-1}w, w \rangle}{N(z)}(A - z)^{-1}w \\ &= z^{j-1}(A - z)^{-1}w + A^{j-2}w + zA^{j-3}w + \cdots + z^{j-2}w \\ &\quad - z^{j-1} \frac{\langle (A - z)^{-1}w, w \rangle}{N(z)}(A - z)^{-1}w \\ &\quad - \frac{\langle A^{j-2}w + zA^{j-3}w + \cdots + z^{j-2}w, w \rangle}{N(z)}(A - z)^{-1}w. \end{aligned}$$

Here the last summand vanishes because of (4.3), and it follows that

$$\begin{aligned} (\widehat{A} - z)^{-1}w_j &= A^{j-2}w + zA^{j-3}w + \cdots + z^{j-2}w \\ &= w_{j-1} + zw_{j-2} + \cdots + z^{j-2}w_1. \end{aligned}$$

We have

$$\mathcal{L} = \text{span}\{w_1, w_2, \dots, w_{m+q}\} \subset \widehat{\mathcal{L}}. \quad (4.9)$$

Since  $w_{m+q} = A^{m-1+q}w \notin \text{dom } A$  and  $\text{dom } \widehat{A} \subset \text{dom } A$  (see (3.6)) we have that  $w_{m+q} \notin \text{dom } \widehat{A}$ . This shows that the chain  $w_1, w_2, \dots, w_{m+q}$  of  $\widehat{A}$  at  $z = \infty$  is maximal and hence that the span of this chain coincides with the root space  $\widehat{\mathcal{L}}$ , that is, in (4.9) equality prevails.

It remains to show that  $u_0 := P_0u \notin \text{dom } \widehat{A}$  if  $m = 0$ . To this end we observe that with the decomposition  $\widehat{\Pi}_\kappa = \mathcal{H}_0 \oplus \widehat{\mathcal{L}}$ ,  $\widehat{\mathcal{L}}$  being a regular subspace of  $\Pi_\kappa$  as  $m = 0$ , the self-adjoint relation  $\widehat{A}$  induces a self-adjoint operator  $\widehat{A}_0$  in  $\mathcal{H}_0$ . In fact, we can write

$$\widehat{A} = \widehat{A}_0 \oplus T^{-1}, \quad (4.10)$$

where  $\widehat{A}_0 = P_0\widehat{A}|_{\mathcal{H}_0}$  is self-adjoint (see, for example, [8, Theorem 3.3]) and  $T$  is the shift operator on  $\widehat{\mathcal{L}}$  such that  $Tw_1 = 0$ ,  $Tw_j = w_{j-1}$ ,  $j = 2, \dots, q$ . That  $\widehat{A}_0$  is an

operator can be seen as follows. If  $\{0, x\} \in \widehat{A}_0$  then there exists a  $y \in \Pi_\kappa$  such that  $\{0, y\} \in \widehat{A}$  and  $P_0 y = x$ . But then  $y$  is a multiple of  $w$ , hence  $x = Py = 0$ . From (4.10) it follows that

$$(\widehat{A} - z)^{-1} = (\widehat{A}_0 - z)^{-1} \oplus T(I - zT)^{-1} \quad (4.11)$$

and therefore

$$\langle (\widehat{A} - z)^{-1} u, u \rangle = \langle (\widehat{A}_0 - z)^{-1} u_0, u_0 \rangle + q(z),$$

where  $q(z)$  is a polynomial of degree  $\leq q - 2$ . Now the operator representation of  $\widehat{N}(z)$  in (iii) becomes

$$\widehat{N}(z) = (z - z_0^*) \langle (I + (z - z_0)(\widehat{A}_0 - z)^{-1}) u_0, u_0 \rangle + p(z), \quad z \in \rho(\widehat{N}),$$

with some polynomial  $p(z)$  of degree  $\leq q$ . Assuming to the contrary that  $u_0 \in \text{dom } \widehat{A}$ , then  $u_0 \in \text{dom } \widehat{A}_0$  and setting  $v_0 := (\widehat{A}_0 - z_0) u_0$ , this formula becomes

$$\widehat{N}(z) = \langle (\widehat{A}_0 - z)^{-1} v_0, v_0 \rangle + p(z), \quad z \in \rho(N),$$

with some polynomial  $p(z)$ . Then, according to the reasoning in (iv)  $\Rightarrow$  (ii), in the second relation in (4.5) we get the sign  $<$ , which according to Lemma 4.1 implies  $w \in \text{dom } A^q$ , a contradiction.

(iii)  $\Rightarrow$  (iv): Again we take  $z_0 = i$ . Since  $\infty$  is the only pole of nonpositive type or generalized pole of nonpositive type of  $\widehat{N}(z)$ , by [2,17]  $\widehat{N}(z)$  has either an irreducible representation

$$\widehat{N}(z) = (1 + z^2)^{\widehat{m}} \widehat{N}_0(z) + p(z)$$

with an integer  $\widehat{m} > 0$ , a real polynomial  $p(z)$  and a Nevanlinna function  $\widehat{N}_0(z)$  with properties (1.7), or a representation

$$\widehat{N}(z) = \widehat{N}_0(z) + p(z)$$

with a Nevanlinna function  $\widehat{N}_0(z)$  and a real polynomial  $p(z)$ . In the first case, since we have proved already that (iv)  $\Rightarrow$  (i),  $\widehat{m}$  coincides with the dimension of the isotropic subspace of the root space of  $\widehat{A}$  at  $\infty$  and hence  $\widehat{m} = m$ . In the second case, if the function  $\widehat{N}_0(z)$  would not have properties (1.5) then it could be chosen to admit a representation

$$\widehat{N}_0(z) = \int_{\mathbb{R}} \frac{d\sigma(t)}{t - z}$$

with a nondecreasing bounded function  $\sigma(t)$ . Applying the Stieltjes–Liřsic inversion formula to the relation

$$\widehat{N}(z) = \widehat{N}(-i) + (z+i) \langle (I + (z-i)(\widehat{A}-z)^{-1})u, u \rangle = \int_{\mathbb{R}} \frac{d\sigma(t)}{t-z} + p(z)$$

for  $\gamma$  large enough we obtain

$$\int_{|t|>\gamma} (t^2+1) d \langle \widehat{E}(t)u, u \rangle = \int_{|t|>\gamma} d\sigma(t) < \infty,$$

which yields  $P_0 u \in \text{dom } \widehat{A}$ , a contradiction. Finally, formula (4.7) follows directly from (1.16) and the relation  $q = \max\{\ell - 2m, 0\}$ .  $\square$

**Remark 4.4.** That (i) of Theorem 4.2 implies  $u_0 = P_0 u \notin \text{dom } \widehat{A}$  if  $m = 0$  in (iii) can also be proved using Krein’s formula (3.3), (3.6) and the fact that  $u$  is cyclic for  $\widehat{A}$ . Indeed, from the definition of  $\widehat{A}_0$  and (3.6) we have that

$$\text{dom } \widehat{A}_0 = \text{dom } \widehat{A} \cap \mathcal{H}_0 \subset \text{dom } A \cap \mathcal{H}_0.$$

We prove the converse inclusion. Let  $x \in \text{dom } A \cap \mathcal{H}_0$ , fix a  $z \in \rho(A)$  and set  $y = (A - z)x$ . Then (3.3) implies

$$(\widehat{A} - z)^{-1}y = (A - z)^{-1}y - \frac{\langle y, \varphi(z^*) \rangle}{N(z)} \varphi(z) = x - \frac{\langle x, w \rangle}{N(z)} \varphi(z) = x,$$

because  $x \perp w$ . Hence  $x \in \text{dom } \widehat{A} \cap \mathcal{H}_0$ . We conclude that

$$\text{dom } A \cap \mathcal{H}_0 = \text{dom } \widehat{A}_0. \quad (4.12)$$

We have  $u = u_0 + \sum_{j=1}^q a_j A^{j-1}w$ , where, since  $u$  is cyclic for  $\widehat{A}$  and by the diagonal representation (4.11) of the resolvent of  $\widehat{A}$ , the coefficient  $a_q \neq 0$ . Hence  $\sum_{j=1}^q a_j A^{j-1}w \notin \text{dom } A$ . As  $u \in \text{dom } A$ , we see that  $u_0 \notin \text{dom } A$ , and then on account of (4.12),  $u_0 \notin \text{dom } \widehat{A}_0$ .

## 5. Rank one perturbation at infinite coupling (2)

In this section we apply Theorem 4.2 to the self-adjoint operator  $H$  with cyclic element  $w$  in  $\Pi_\kappa$  and the relation  $H^\infty$  studied in Section 2. We assume that  $H$  and  $w$  have the same properties as  $A$  and  $w$  in Theorem 4.2(i), that is, we assume that for some integers  $m, q \in \mathbb{N}_0$  with  $m + q > 0$ ,

$$w \in \text{dom } H^{m-1+q} \setminus \text{dom } H^{m+q},$$

the subspace

$$\mathcal{L} := \text{span}\{w, Hw, \dots, H^{m-1}w, H^mw, \dots, H^{m-1+q}w\}$$

has index of nonpositivity  $\kappa$ , and

$$\begin{aligned} \langle H^j w, H^k w \rangle &= 0, \quad 0 \leq j, \quad k \leq m+q-1, \quad j+k \leq 2m+q-2, \\ \langle H^j w, H^k w \rangle &\neq 0, \quad 0 \leq j, \quad k \leq m+q-1, \quad j+k = 2m+q-1. \end{aligned} \quad (5.1)$$

The basis elements of  $\mathcal{L}$  we denote by  $w_j$ :

$$w_j := H^{j-1}w, \quad j = 1, 2, \dots, m+q.$$

In particular,  $\mathcal{L}_0 := \text{span}\{w_1, w_2, \dots, w_m\}$  is the isotropic subspace of  $\mathcal{L}$ ; see Remark 4.3(i). By  $G_{\mathcal{L}}$  we denote the Gram matrix associated with the basis elements  $w_1, w_2, \dots, w_{m+q}$  of  $\mathcal{L}$ :

$$G_{\mathcal{L}} = (g_{ij})_{i,j=0}^{m+q-1}, \quad g_{ij} = \langle H^i w, H^j w \rangle.$$

Then  $G_{\mathcal{L}}$  is the  $(m+q) \times (m+q)$  block matrix

$$G_{\mathcal{L}} := \begin{pmatrix} 0 & 0 \\ 0 & G' \end{pmatrix},$$

in which the zero in the left upper corner stands for the  $m \times m$  zero matrix and the matrix  $G'$  in the right lower corner is the invertible  $q \times q$  Hankel matrix

$$G' := \begin{pmatrix} 0 & 0 & \cdots & 0 & s_{n-1} \\ 0 & 0 & \cdots & s_{n-1} & s_n \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & s_{n-1} & \cdots & s_{n+q-4} & s_{n+q-3} \\ s_{n-1} & s_n & \cdots & s_{n+q-3} & s_{n+q-2} \end{pmatrix}, \quad (5.2)$$

where  $s_j = \langle H^r w, H^s w \rangle$ ,  $j = r+s$ ,  $0 \leq r, s \leq m+q-1$  and  $n = 2m+q$ . If  $q = 0$ , then the matrix  $G_{\mathcal{L}}$  reduces to the  $m \times m$  zero matrix; if  $m = 0$ , then  $G_{\mathcal{L}} = G'$ .

From Section 2 we recall the  $\Pi_{\kappa}$ -valued and the scalar functions

$$\begin{aligned} \varphi(z) &= (H-z)^{-1}w, \quad Q(z) = \langle (H-z)^{-1}w, w \rangle, \\ \varphi^{\infty}(z) &= Q(z)^{-1}\varphi(z), \quad Q^{\infty}(z) = -Q(z)^{-1}, \end{aligned} \quad (5.3)$$

see (2.2) and Theorem 2.1. According to (5.1) and the assumptions preceding it, the function  $Q(z)$  has the same properties as  $N(z)$  in Theorem 4.2(i), and hence it has the

same asymptotic behavior as  $N(z)$  in Theorem 4.2(ii). In this section we focus on the properties of  $Q^\infty(z)$  which are the same as  $\widehat{N}(z)$  in Theorem 4.2(iii) and (iv):  $Q^\infty(z)$  belongs to the class  $\mathcal{N}_\kappa^\infty$  and admits the irreducible (hence unique) representation:

$$Q^\infty(z) = c(z)^m Q_0(z) + p_\ell(z), \quad c(z) = (z - z_0)(z - z_0^*), \quad (5.4)$$

where  $z_0 \in \mathbb{C} \setminus \mathbb{R}$ ,  $m \in \mathbb{N}_0$ ,  $Q_0(z) \in \mathcal{N}_0$  satisfies (1.7),  $p_\ell(z)$  is a real polynomial of degree  $\ell$  and the relation between  $q$ ,  $\ell$ , and  $m$  is given by  $q = \max\{\ell - 2m, 0\}$ . Because of Theorem 2.1(ii), we may assume that  $H^\infty$  is the relation appearing in the operator representation for  $Q^\infty(z)$ :

$$Q^\infty(z) = Q^\infty(z_0^*) + (z - z_0^*) \langle (I + (z - z_0)(H^\infty - z)^{-1})u, u \rangle, \quad z \in \rho(H^\infty),$$

where  $u = \varphi^\infty(z_0)$  is a cyclic element for  $H^\infty$  (in the sequel we will denote this element also by  $u_1$ ). By the identification mentioned at the end of Theorem 4.2, we may also assume that  $\mathcal{L}$  is the root space of  $H^\infty$  at  $z = \infty$  and that the elements  $w = w_1, w_2, \dots, w_{m+q}$  form a Jordan chain for  $H^\infty$  at  $z = \infty$ , that is, with  $R^\infty(z) = (H^\infty - z)^{-1}$ ,

$$R^\infty(z)w = 0,$$

$$R^\infty(z)w_j = w_{j-1} + zw_{j-2} + \dots + z^{j-2}w, \quad j = 2, 3, \dots, m+q; \quad (5.5)$$

see Remark 4.3(ii).

In the following we construct a decomposition of the space  $\Pi_\kappa$  and the matrix decomposition of the resolvent operator  $R^\infty(z)$  relative to this decomposition; see (5.10) and (5.11) below. We assume  $m > 0$ , the case  $m = 0$  is simpler and we will indicate the differences between this case and the case  $m > 0$  later. With  $z_0 \in \mathbb{C} \setminus \mathbb{R}$  ( $\subset \rho(Q^\infty)$ ) and the monomials

$$b_k(z) := (z - z_0)^k, \quad k = 0, 1, \dots, m,$$

we introduce the elements  $u_k \in \Pi_\kappa$ ,  $k = 1, 2, \dots, m$ , and the function  $\phi(z)$  via the expansion of

$$\varphi^\infty(z) = \varphi^\infty(z_0) + (z - z_0)R^\infty(z)\varphi^\infty(z_0)$$

at  $z = z_0$ :

$$\begin{aligned} \varphi^\infty(z) &= \sum_{k=1}^m b_{k-1}(z)R^\infty(z)^{k-1}\varphi^\infty(z_0) + b_m(z)R^\infty(z)R^\infty(z_0)^{m-1}\varphi^\infty(z_0) \\ &= \sum_{k=1}^m b_{k-1}(z)u_k + b_m(z)\phi(z), \end{aligned}$$

that is,

$$u_k = \frac{1}{(k-1)!} \frac{d^{k-1}}{dz^{k-1}} \varphi^\infty(z) \Big|_{z=z_0} = R^\infty(z_0)^{k-1} \varphi^\infty(z_0), \quad k = 1, 2, \dots, m,$$

so that

$$u_1 = \varphi^\infty(z_0) = u, \quad u_k = R^\infty(z_0)^{k-1} u, \quad k = 1, 2, 3, \dots, m,$$

and

$$\begin{aligned} \phi(z) &= \frac{1}{b_m(z)} \left( \varphi^\infty(z) - \sum_{k=1}^m b_{k-1}(z) u_k \right) \\ &= R^\infty(z) R^\infty(z_0)^{m-1} \varphi^\infty(z_0) = R^\infty(z) u_m. \end{aligned} \quad (5.6)$$

Note that if  $m = 0$  then  $\phi(z) = \varphi^\infty(z)$ . Finally, we form the subspace

$$\mathcal{M} := \text{span}\{u_1, u_2, \dots, u_m\} \quad (5.7)$$

and show that it is skewly linked with the isotropic subspace  $\mathcal{L}^0$  of  $\mathcal{L}$ . Here *skewly linked* means that no element of  $\mathcal{M}$  is orthogonal to  $\mathcal{L}^0$  and no element of  $\mathcal{L}^0$  is orthogonal to  $\mathcal{M}$ . Using the definitions of  $\varphi^\infty(z)$  and  $Q(z)$ , we find for  $j = 1, 2, \dots, m+q$ ,

$$\begin{aligned} \langle \varphi^\infty(z), w_j \rangle &= \frac{1}{Q(z)} \langle (H-z)^{-1} w, H^{j-1} w \rangle \\ &= \frac{z}{Q(z)} \langle (H-z)^{-1} w, H^{j-2} w \rangle \\ &= \dots = \frac{z^{j-1}}{Q(z)} \langle (H-z)^{-1} w, w \rangle = z^{j-1}. \end{aligned}$$

It follows that for  $j = 1, 2, \dots, m+q$  and  $k = 1, 2, \dots, m$ ,

$$\langle u_k, w_j \rangle = \binom{j-1}{k-1} z_0^{j-k}, \quad (5.8)$$

in particular,  $\langle u_k, w_j \rangle = 0$  if  $k > j$  and  $= 1$  if  $k = j$ . Define

$$v_j := (H - z_0^*)^{j-1} w, \quad j = 1, 2, \dots, m+q,$$

and consider  $k \in \{1, 2, \dots, m\}$ . On account of (5.8), if  $k > j$  then

$$\langle u_k, v_j \rangle = 0,$$



if  $k < j$  then

$$\begin{aligned}
 \langle u_k, v_j \rangle &= \sum_{\ell=1}^j \binom{j-1}{\ell-1} (-z_0)^{j-\ell} \langle u_k, H^{\ell-1} w \rangle \\
 &= \sum_{\ell=k}^j \binom{j-1}{\ell-1} (-z_0)^{j-\ell} \binom{\ell-1}{k-1} z_0^{\ell-k} \\
 &= \binom{j-1}{k-1} z_0^{j-k} \sum_{\ell=k}^j \binom{j-k}{\ell-k} (-1)^{j-\ell} \\
 &= \binom{j-1}{k-1} z_0^{j-k} \sum_{\ell=0}^{j-k} \binom{j-k}{\ell} (-1)^{j-\ell-k} = \binom{j-1}{k-1} z_0^{j-k} (1-1)^{j-k} = 0,
 \end{aligned}$$

and if  $k = j$  then, as follows from the second equality in these calculations,

$$\langle u_k, v_j \rangle = 1.$$

Hence, since

$$\mathcal{L}^0 = \text{span}\{v_1, v_2, \dots, v_m\},$$

$\mathcal{L}^0$  and  $\mathcal{M}$  are skewly linked, and the bases  $\{v_j\}_{j=1}^m$  in  $\mathcal{L}^0$  and  $\{u_j\}_{j=1}^m$  in  $\mathcal{M}$  are bi-orthonormal. Moreover,  $\mathcal{M}$  is orthogonal to the elements  $v_j$  with  $j = m+1, \dots, m+q$ , and therefore

$$\mathcal{L}' := \text{span}\{v_{m+1}, v_{m+2}, \dots, v_{m+q}\} \quad (5.9)$$

is a regular  $q$ -dimensional subspace of  $\Pi_\kappa$  and  $\mathcal{L} = \mathcal{L}^0 \oplus \mathcal{L}'$ . It follows that  $(\Pi_\kappa, \langle \cdot, \cdot \rangle)$  can be decomposed as

$$\Pi_\kappa = \mathcal{H}_0 \oplus (\mathcal{L}^0 \dot{+} \mathcal{M}) \oplus \mathcal{L}', \quad (5.10)$$

where  $(\mathcal{H}_0, \langle \cdot, \cdot \rangle)$  is a Hilbert subspace (in the sequel the Hilbert inner product  $\langle \cdot, \cdot \rangle$  on  $\mathcal{H}_0$  will also be denoted by  $\langle \cdot, \cdot \rangle_0$ ). Since

$$R^\infty(z)\mathcal{L} \subset \mathcal{L}$$

and  $R^\infty(z)^* = R^\infty(z^*)$ , we have

$$R^\infty(z)\mathcal{L}^\perp \subset \mathcal{L}^\perp, \quad \mathcal{L}^\perp = \mathcal{H}_0 \oplus \mathcal{L}^0,$$

and hence

$$R^\infty(z)\mathcal{L}^0 \subset \mathcal{L}^0, \quad \mathcal{L}^0 = \mathcal{L} \cap \mathcal{L}^\perp.$$

These three inclusions imply the following structure of the block matrix of  $R^\infty(z)$  with respect to decomposition (5.10):

$$R^\infty(z) = \begin{pmatrix} R_{00}(z) & 0 & R_{02}(z) & 0 \\ R_{10}(z) & R_{11}(z) & R_{12}(z) & R_{13}(z) \\ 0 & 0 & R_{22}(z) & 0 \\ 0 & 0 & R_{32}(z) & R_{33}(z) \end{pmatrix}. \quad (5.11)$$

If  $m = 0$ , then  $q \geq 1$ ,  $\mathcal{M} = \mathcal{L}^0 = \{0\}$ ,  $\mathcal{L}' = \mathcal{L}$ , decomposition (5.10) becomes  $\Pi_\kappa = \mathcal{H}_0 \oplus \mathcal{L}$ , and with respect to this decomposition  $R^\infty(z)$  has the diagonal form

$$R^\infty(z) = \begin{pmatrix} R_{00}(z) & 0 \\ 0 & R_{33}(z) \end{pmatrix}. \quad (5.12)$$

If  $q = 0$ , then  $m = \kappa \geq 1$ ,  $\mathcal{L}^0 = \mathcal{L}$ ,  $\mathcal{L}' = \{0\}$ , decomposition (5.10) becomes  $\Pi_\kappa = \mathcal{H}_0 \oplus (\mathcal{L} \dot{+} \mathcal{M})$ , and relative to this decomposition  $R^\infty(z)$  has the block matrix representation

$$R^\infty(z) = \begin{pmatrix} R_{00}(z) & 0 & R_{02}(z) \\ R_{10}(z) & R_{11}(z) & R_{12}(z) \\ 0 & 0 & R_{22}(z) \end{pmatrix}. \quad (5.13)$$

We denote by  $P_0$  the orthogonal projection in  $\Pi_\kappa$  onto  $\mathcal{H}_0$ . Formulas (5.11)–(5.13) show that  $H^\infty$  induces a self-adjoint operator  $A_0$  in  $\mathcal{H}_0$  by the formula  $(A_0 - z)^{-1} = P_0(H^\infty - z)^{-1}|_{\mathcal{H}_0}$ . That  $A_0$  is densely defined can be seen as follows: Assume  $x \in \mathcal{H}_0 \ominus \text{dom } A_0$ . Then  $\{0, x\} \in A_0^* = A_0$  and hence  $(A_0 - z)^{-1}x = 0$  for all  $z \in \rho(A_0)$ ; we fix one such  $z$ . In terms of the matrix decomposition (5.11) of  $R^\infty(z)$  we have that  $R_{00}(z)x = 0$ , hence  $R^\infty(z)x = R_{10}(z)x \in \mathcal{L}^0 \subset \mathcal{L}$ . As  $\mathcal{L}$  is the root space of  $H^\infty$  at  $z = \infty$ , there is an integer  $n \geq 0$  such that  $R^\infty(z)^n x = 0$ , and therefore  $x \in \mathcal{L} \cap \mathcal{H}_0 = \{0\}$ , that is,  $x = 0$ .

In part (iii) of the next theorem the space  $\mathcal{H}_{-1}$  is the space with negative norm associated with the operator  $A_0$  in  $\mathcal{H}_0$  (see Section 1.4).

**Theorem 5.1.** *Let  $H$  be a self-adjoint operator in a Pontryagin space  $\Pi_\kappa$  and let  $w \in \Pi_\kappa$  be an element which is cyclic for  $H$ . Assume that*

$$w \in \text{dom } H^{m+q-1} \setminus \text{dom } H^{m+q}$$

*for some integers  $m, q \in \mathbb{N}_0$ ,  $m + q > 0$ , that the subspace*

$$\mathcal{L} := \text{span}\{w, Hw, \dots, H^{m-1}w, H^m w, \dots, H^{m+q-1}w\}$$

has index of nonpositivity  $\kappa$ , and that

$$\begin{aligned}\langle H^j w, H^k w \rangle &= 0, \quad 0 \leq j, \quad k \leq m+q-1, \quad j+k \leq 2m+q-2, \\ \langle H^j w, H^k w \rangle &\neq 0, \quad 0 \leq j, \quad k \leq m+q-1, \quad j+k = 2m+q-1.\end{aligned}\quad (5.14)$$

Then the infinite coupling  $H^\infty$  of  $H$  with  $w$  has the following properties:

- (i) The subspace  $\mathcal{L}$  is the root space of  $H^\infty$  at  $z = \infty$  and the elements  $w, Hw, \dots, H^{m-1}w, H^m w, \dots, H^{m+q-1}w$  form a corresponding Jordan chain. If  $m = 0$ , then  $\mathcal{L}$  is nondegenerated; if  $m \geq 1$ , then  $\mathcal{L}$  is degenerated, the subspace

$$\mathcal{L}^0 = \text{span}\{v_1, v_2, \dots, v_m\}, \quad v_j = (H - z_0^*)^{j-1}w, \quad j = 1, 2, \dots, m+q,$$

is the isotropic part of  $\mathcal{L}$ , the subspace  $\mathcal{M}$  from (5.7):

$$\mathcal{M} = \text{span}\{u_1, u_2, \dots, u_m\}, \quad u_k = R^\infty(z_0)^{k-1} \varphi^\infty(z_0), \quad k = 1, 2, \dots, m,$$

is skewly linked with  $\mathcal{L}^0$  and orthogonal to the subspace

$$\mathcal{L}' = \text{span}\{v_{m+1}, v_{m+2}, \dots, v_{m+q}\}.$$

With respect to decomposition (5.10) of the space  $\Pi_\kappa$  the resolvent of the self-adjoint relation  $H^\infty$  admits the representation (5.11) where  $R_{00}(z)$  is the resolvent of a self-adjoint operator  $A_0$  in the Hilbert space  $\mathcal{H}_0$ .

- (ii) The restriction

$$S_0 = A_0|_{\{f \in \text{dom } A_0 \mid \langle (A_0 - z_0^*)f, \varphi_0(z_0) \rangle_0 = 0\}}$$

of  $A_0$  is a densely defined symmetric operator in  $\mathcal{H}_0$ , the function

$$\varphi_0(z) = \frac{1}{(z - z_0)^m} P_0 \varphi^\infty(z), \quad z \in \mathbb{C} \setminus \mathbb{R},$$

is a defect function for  $S_0$  and  $A_0$ , and the function  $Q_0(z)$  from (5.4) is a  $Q$ -function for  $S_0$  and  $A_0$ :  $Q_0(z) \sim S_0, A_0$  in  $\mathcal{H}_0$ .

- (iii) The defect function  $\varphi_0(z)$  can be written as

$$\varphi_0(z) = (A_0 - z)^{-1} \chi_{-1}$$

for some generalized element  $\chi_{-1} \in \mathcal{H}_{-1} \setminus \mathcal{H}_0$ . With the function  $\sigma(t)$  in the irreducible integral representation (1.15) for  $Q^\infty(z)$  it holds

$$\langle (A_0 - z)^{-1} \chi_{-1}, (A_0 - \zeta)^{-1} \chi_{-1} \rangle_0 = \int_{\mathbb{R}} \frac{d\sigma(t)}{(t - z)(t - \zeta^*)}, \quad z, \zeta \in \mathbb{C} \setminus \mathbb{R}.$$

**Proof.** (i) These statements have been proved before the theorem.

(ii) By (5.6) we have that  $\varphi_0(z) = P_0\phi(z)$  and hence

$$\phi(z) = \varphi_0(z) + \sum_{j=1}^{m+q} a_j(z)H^{j-1}w + \sum_{j=1}^m c_j(z)u_j. \quad (5.15)$$

We claim (1)  $c_j(z) = 0, j = 1, \dots, m$  and (2)  $a_{m+1}(z), \dots, a_{m+q}(z)$  are polynomials in  $z$  of degree  $\leq q-1$ . If  $m = 0$  part (1) and if  $q = 0$  part (2) of the claim should be discarded. To prove the claim we use (5.5). For (1) we take the inner product of the elements of both sides of (5.15) with  $v_k = (H - z_0^*)^{k-1}w$ . The inner product of the function on the right-hand side of (5.15) with  $v_k$  is equal to  $c_k(z)$ , whereas the inner product of  $\phi(z)$  on the left-hand side with  $v_k$  equals

$$\langle \phi(z), v_k \rangle = \langle u_m, R^\infty(z^*)v_k \rangle = 0;$$

the first equality holds because of (5.6) and the second equality holds because of  $R^\infty(z^*)v_1 = R^\infty(z^*)w = 0$  and

$$R^\infty(z^*)v_k \in \text{span}\{w, Hw, \dots, H^{k-2}w\}, \quad k = 2, \dots, m.$$

We conclude that  $c_k(z) = 0, k = 1, 2, \dots, m$ . To verify (2) we take the inner product of the elements on both sides of (5.6) with  $H^{k-1}w, k = 1, 2, \dots, m+q$ . We obtain

$$\begin{pmatrix} \langle \phi(z), w \rangle \\ \langle \phi(z), Hw \rangle \\ \vdots \\ \langle \phi(z), H^{m+q-1}w \rangle \end{pmatrix} = G_{\mathcal{L}} \begin{pmatrix} a_1(z) \\ a_2(z) \\ \vdots \\ a_{m+q}(z) \end{pmatrix}.$$

The first  $m$  entries of the vectors on both sides of the equality are equal to 0, and so we are left with

$$\begin{pmatrix} \langle \phi(z), H^m w \rangle \\ \langle \phi(z), H^{m+1} w \rangle \\ \vdots \\ \langle \phi(z), H^{m+q-1} w \rangle \end{pmatrix} = G' \begin{pmatrix} a_{m+1}(z) \\ a_{m+2}(z) \\ \vdots \\ a_{m+q}(z) \end{pmatrix}.$$

The matrix  $G'$  is invertible and for  $s = 0, 1, \dots, q-1$  we have, using (5.6), that

$$\begin{aligned} \langle \phi(z), H^{m+s} w \rangle &= \langle u_m, R^\infty(z^*)H^{m+s} w \rangle \\ &= \langle u_m, H^{m+s-1} w + z^* H^{m+s-2} w + \dots + z^{*(m+s-1)} w \rangle \\ &= \langle u_m, H^{m+s-1} w + z^* H^{m+s-2} w + \dots + z^{*s} H^{m-1} w \rangle \end{aligned}$$

is a polynomial of degree  $s$  (with leading coefficient 1), which readily implies claim (2). Hence

$$\phi(z) = \varphi_0(z) + \sum_{j=1}^{m+q} a_j(z) H^{j-1} w \in \mathcal{H}_0 \oplus \mathcal{L} \quad (5.16)$$

and the degrees of the polynomials  $a_j(z)$ ,  $j = m+1, \dots, m+q$ , are all  $\leq q-1$ .

We show that  $\varphi_0(z)$  satisfies a relation of form (1.1). Let  $z, \zeta \in \mathbb{C} \setminus \mathbb{R}$ . Then on account of (5.6),

$$\begin{aligned} \varphi_0(z) - \varphi_0(\zeta) &= P_0(R^\infty(z) - R^\infty(\zeta))u_m \\ &= (z - \zeta)P_0R^\infty(z)R^\infty(\zeta)u_m = (z - \zeta)P_0R^\infty(z)\phi(\zeta) \\ &= (z - \zeta)P_0R^\infty(z)P_0\phi(\zeta) = (z - \zeta)(A_0 - z)^{-1}\varphi_0(\zeta). \end{aligned}$$

For the last equality we used that  $P_0R^\infty(z)|_{\mathcal{H}_0} = (A_0 - z)^{-1}$  and for the equality before that we used that

$$P_0R^\infty(z)\phi(\zeta) = P_0R^\infty(z)P_0\phi(\zeta),$$

which follows from the matrix representation (5.11) of  $R^\infty(z)$  and the fact that  $\phi(\zeta) \in \mathcal{H}_0 \oplus \mathcal{L}^0 \oplus \mathcal{L}'$ , see (5.16). Hence  $\varphi_0(z)$  is a defect function for the symmetric operator  $S_0$  as defined in (ii) and its self-adjoint extension  $A_0$ . We show that  $S_0$  is densely defined, or equivalently that

$$\varphi_0(z) \notin \text{dom } A_0, \quad z \in \rho(A_0).$$

As  $\varphi_0(z)$  is a defect function for  $S_0$  and  $A_0$ , it suffices to prove this for only one  $z \in \rho(A_0)$ . We consider two cases:

Case  $m > 0$ : Then (5.6) and (5.16) imply

$$R^\infty(z)u_m - \varphi_0(z) = \phi(z) - \varphi_0(z) \in \mathcal{L}.$$

If  $\varphi_0(z) \in \text{dom } A_0$ , then it can be written as  $\varphi_0(z) = (A_0 - z)^{-1}\xi(z)$  for some  $\xi(z) \in \mathcal{H}_0$ , and hence, because of (5.11),

$$\varphi_0(z) - R^\infty(z)\xi(z) \in \mathcal{L}_0.$$

It follows that  $R^\infty(z)(u_m - \xi(z))$  and, as  $\mathcal{L}$  is the root subspace of  $H^\infty$  at  $z = \infty$ , also  $u_m - \xi(z)$  belongs to  $\mathcal{L}$ . Hence

$$u_m \in \mathcal{M} \cap (\mathcal{H}_0 \oplus \mathcal{L}) = \{0\}.$$

This implies that  $R^\infty(z_0)^m u_1 = u_m = 0$  and hence  $u_1 \in \mathcal{M} \cap \mathcal{L} = \{0\}$ , a contradiction, as  $u_1$  is a cyclic element for  $H^\infty$ .

Case  $m = 0$ : By Theorem 4.2(iii) we have  $\varphi_0(z_0) = u_0 = P_0 u \notin \text{dom } H^\infty$  and from

$$\text{dom } H^\infty \cap \mathcal{H}_0 = \text{dom } A_0,$$

which follows from  $P_0 H^\infty|_{\mathcal{H}_0} = A_0$ , we conclude that  $\varphi_0(z_0) \notin \text{dom } A_0$ .

We now prove the second statement of (ii). Again we first consider the case that  $m > 0$ . Recall that

$$\begin{aligned} Q^\infty(z) &= Q^\infty(z_0^*) + (z - z_0^*) \langle \varphi^\infty(z), \varphi^\infty(z_0) \rangle \\ &= Q^\infty(z_0^*) + (z - z_0^*) \langle u_1, u_1 \rangle + (z - z_0^*)(z - z_0) \langle R^\infty(z) u_1, u_1 \rangle. \end{aligned}$$

Hence if we define

$$Q_1(z) := \langle R^\infty(z) u_m, u_m \rangle = \langle R^\infty(z) R^\infty(z_0)^{m-1} R^\infty(z_0^*)^{m-1} u_1, u_1 \rangle,$$

then

$$Q^\infty(z) = c(z)^m Q_1(z) + p(z),$$

where

$$\begin{aligned} p(z) &= Q^\infty(z_0^*) + (z - z_0^*) \langle u_1, u_1 \rangle \\ &\quad + \langle [c(z) R^\infty(z) - c(z)^m R^\infty(z) R^\infty(z_0)^{m-1} R^\infty(z_0^*)^{m-1}] u_1, u_1 \rangle \end{aligned}$$

is a polynomial of degree at most  $2m - 1$ , because the expression in the square brackets is an operator polynomial of degree at most  $2m - 1$ . Since  $Q^\infty(z)^* = Q^\infty(z^*)$  and  $Q_1(z)^* = Q_1(z^*)$ , the polynomial  $p(z)$  is real. The function  $Q_1(z)$  can also be written as

$$Q_1(z) = \langle u_m, \phi(z_0) \rangle + (z - z_0^*) \langle \phi(z), \phi(z_0) \rangle$$

and inserting expression (5.16) for  $\varphi(z)$  into this formula we obtain the equality

$$Q_1(z) = N_0(z) + q(z), \tag{5.17}$$

in which

$$N_0(z) := a - i(\text{Im } z_0) \langle \varphi_0(z_0), \varphi_0(z_0) \rangle_0 + (z - z_0^*) \langle \varphi_0(z), \varphi_0(z_0) \rangle_0$$

is a Nevanlinna function with  $a \in \mathbb{R}$  such that  $\text{Re } N_0(i) = 0$ , and

$$q(z) := \langle u_m, \phi(z_0) \rangle - a + (z - z_0^*) \left\langle \sum_{j=m+1}^{m+q} a_j(z) H^{j-1} w, \sum_{j=m+1}^{m+q} a_j(z_0) H^{j-1} w \right\rangle$$

is a real polynomial of degree  $\leq q$ . Combining these formulas we obtain

$$Q^\infty(z) = c(z)^m N_0(z) + \tilde{p}(z), \quad (5.18)$$

where  $\tilde{p}(z) = c(z)^m q(z) + p(z)$  is a real polynomial of degree  $\leq 2m + q$ . In a similar way it can be shown that this formula also holds when  $m = 0$ . From the definition of  $N_0(z)$  it follows that  $N_0(z) \sim S_0, A_0$  in  $\mathcal{H}_0$  provided  $\varphi_0(z)$  spans  $\mathcal{H}_0$ . But this follows from the fact that  $\varphi^\infty(z)$  spans  $\Pi_\kappa$ . Since  $S_0$  is densely defined in  $\mathcal{H}_0$ , we have that  $N_0(z)$  satisfies (1.7) and (5.18) is an irreducible representation of  $Q^\infty(z)$ . Comparing this representation and the representation (5.4) for  $Q^\infty(z)$ , we get  $Q_0(z) = N_0(z)$  (and  $p_\ell(z) = \tilde{p}(z)$ ) and hence  $Q_0(z) \sim S_0, A_0$  in  $\mathcal{H}_0$ .

(iii) As  $\varphi_0(z)$  is the defect function of  $S_0$  and  $A_0$  we have

$$\varphi_0(z) - \varphi_0(\zeta) = (z - \zeta)(A_0 - z)^{-1} \varphi_0(\zeta),$$

and hence

$$(A_0 - z)\varphi_0(z) - (A_0 - \zeta)\varphi_0(\zeta) = (A_0 - z)(\varphi_0(z) - \varphi_0(\zeta)) - (z - \zeta)\varphi_0(\zeta) = 0.$$

This equality holds in  $\mathcal{H}_{-1}$  and not in  $\mathcal{H}_0$ , because  $\varphi_0(z) \notin \text{dom } A_0$ . We see that  $(A_0 - z)\varphi_0(z)$  belongs to  $\mathcal{H}_{-1} \setminus \mathcal{H}_0$ , does not depend on  $z \in \rho(A_0)$ , and defines a generalized element  $\chi_{-1} \in \mathcal{H}_{-1} \setminus \mathcal{H}_0$  such that  $\varphi_0(z) = (A_0 - z)^{-1} \chi_{-1}$ . The cyclicity of  $\chi_{-1}$  in  $\mathcal{H}_{-1}$  is equivalent to the property

$$\mathcal{H}_0 = \overline{\text{span}}\{\varphi_0(z) \mid z \in \rho(A_0)\}.$$

The integral formula at the end of the theorem follows from the equality

$$\langle \varphi_0(z), \varphi_0(\zeta) \rangle_0 = \frac{Q_0(z) - Q_0(\zeta)}{z - \zeta^*}. \quad \square$$

**Remark 5.2.** Under the assumptions of Theorem 5.1, set  $n = 2m + q$ .

- (a) If  $n$  is odd and  $\langle H^{\frac{n-1}{2}} w, H^{\frac{n-1}{2}} w \rangle < 0$ , then  $\kappa = \frac{n+1}{2}$ , the subspace  $\text{span}\{w, Hw, \dots, H^{\kappa-1} w\}$  is a maximal nonpositive subspace of  $\mathcal{L}$ , and if  $\kappa > 1$ , the subspace  $\text{span}\{w, Hw, \dots, H^{\kappa-2} w\}$  is a maximal neutral subspace of  $\mathcal{L}$ .
- (b) In all other cases  $\kappa = \left\lfloor \frac{n}{2} \right\rfloor$  and the subspace  $\text{span}\{w, Hw, \dots, H^{\kappa-1} w\}$  is a maximal neutral subspace of  $\mathcal{L}$ .

To substantiate these statements, we first note that with  $n = 2m + q$  the formula (4.7) for  $\kappa$  can be rewritten as

$$\kappa = \begin{cases} \frac{n+1}{2} & \text{if } n \text{ odd, } s_{n-1} < 0, \\ \left\lfloor \frac{n}{2} \right\rfloor & \text{otherwise.} \end{cases}$$

Denote by  $G_r = (g_{ij})_{i,j=0}^{r-1}$  the  $r \times r$  Gram matrix associated with the  $r$  basis elements  $w, Hw, \dots, H^{r-1}w$  of  $\mathcal{L}$ :

$$g_{ij} = \langle H^j w, H^i w \rangle, \quad i, j = 0, 1, \dots, r-1.$$

Then, for example,  $G_{m+q} = G_{\mathcal{L}}$ . To prove (a) and (b) one looks for the largest integer  $r \geq 1$  such that either  $G_r = 0$ , or  $G_r \leq 0$  and  $G_r \neq 0$ . Because of the block form of the matrix  $G_{\mathcal{L}}$  and the triangular form of  $G'$ , the latter occurs precisely when  $\langle H^{r-1}w, H^{r-1}w \rangle = s_{n-1}$  and  $s_{n-1} < 0$ . Then  $n = 1 + 2(r-1)$  is odd,  $\kappa = (n+1)/2 = r$  and  $G_{r-1} = 0$ . This readily implies (a). Statement (b) can be obtained in a similar way.

**Remark 5.3.** The generalized element  $\chi_{-1} \in \mathcal{H}_{-1} \setminus \mathcal{H}_0$  in Theorem 5.1(iii) is connected with the Nevanlinna function  $Q_0(z)$  and the function  $\sigma(t)$  through the formula

$$\langle (A_0 - z)^{-1} \chi_{-1}, (A_0 - z^*)^{-1} \chi_{-1} \rangle_0 = \frac{d}{dz} Q_0(z) = \int_{\mathbb{R}} \frac{d\sigma(t)}{(t-z)^2}, \quad z \in \mathbb{C} \setminus \mathbb{R},$$

compare with [14]. This relation shows that  $\chi_{-1}$  is independent of the reference point  $z_0$  in representation (1.3) for the function  $Q_0(z)$ . That  $\chi_{-1}$  belongs to  $\mathcal{H}_{-1} \setminus \mathcal{H}_0$  is equivalent to  $Q_0(z)$  satisfying (1.5). The irreducible representation (5.4), decomposition (5.10), and hence also the element  $\chi_{-1}$  depend on the choice of the point  $z_0$  (more generally on the choice of the subspace  $\mathcal{M}$  in (5.10)). This fact was explained in [10, Section 6]. There and in the  $\Pi_{\kappa}$  setting of this paper when  $m > 0$  the role of  $\chi_{-1}$  is played by the generalized element

$$\chi := (A_0 - z_0)^m \chi_{-1},$$

which belongs to the space  $\mathcal{H}_{-m-1} \setminus \mathcal{H}_m$ . Indeed,  $\chi$  is connected with the function  $Q^{\infty}(z)$  through the formula

$$\langle (A_0 - z)^{-m-1} \chi, (A_0 - z^*)^{-m-1} \chi \rangle_0 = \frac{1}{(2m+1)!} ((Q^{\infty})(z) - p(z))^{(2m+1)}, \quad (5.19)$$

which can be obtained by differentiating the functions on both sides of the equality

$$\begin{aligned} Q^{\infty}(z) - p(z) &= (z - z_0)^m (z - z_0^*)^m Q_0(z) \\ &= (z - z_0)^m (z - z_0^*)^m (Q_0(z_0^*) \\ &\quad + (z - z_0^*) \langle (A_0 - z)^{-1} \chi_{-1}, (A_0 - z)^{-1} \chi_{-1} \rangle_0 \end{aligned}$$

$2m+1$  times with respect to  $z$ . The right-hand side of (5.19) is independent of the choice of  $z_0$ . If in (5.19) we substitute the irreducible representation (5.4) for  $Q^{\infty}(z)$



we obtain

$$\langle (A_0 - z)^{-m-1} \chi, (A_0 - z^*)^{-m-1} \chi \rangle_0 = \int_{\mathbb{R}} \frac{d\sigma_{\infty}(t)}{(t - z)^{2(m+1)}}, \quad z \in \mathbb{C} \setminus \mathbb{R},$$

in which  $d\sigma_{\infty}(t) := |t - z_0|^{2m} d\sigma(t)$ . Now limit (2.16) can be specified as follows:

$$\lim_{\alpha \rightarrow \infty} \alpha^2 \int_{\Delta} \frac{d\sigma_{\alpha}(t)}{r_{\alpha}(t)(t - z_0)(t - z_0^*)} = -\frac{1}{2\pi i} \int'_{\Gamma_{\Delta}} \frac{Q^{\infty}(z) dz}{(z - z_0)(z - z_0^*)} = \int_{\Delta} \frac{d\sigma_{\infty}(t)}{(t - z_0)(t - z_0^*)},$$

where the interval  $\Delta$  is such that  $\sigma_{\infty}(t)$  is continuous in the boundary points of  $\Delta$ . This is the analog of [14, Theorem 4(iii)] in an indefinite setting.

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### Further reading

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